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A HEALTH AND ENVIRONMENTAL EFFECTS DATA BASE ASSESSMENT
OF U.S. ARMY WASTE MATERIAL

Final Report

PHASE II REPORT

by

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Substances used by the U.S. Army on a regular basis in accomplishing their missions of training, defense and weapons development have a wide range of uses, storage and disposal methods. Humans and the environment may be exposed to them in varying amounts. Proper research planning requires knowledge of gaps in health and environmental data on those compounds. CARLTECH was contracted to develop a data base on health and		

environmental effects of waste materials generated by the U.S. Army.

The project was divided into two phases:

Phase I which consisted of identification of Army-unique materials for inclusion in the data base.

Phase II which consisted of researching, aggregating and reporting data on physical, chemical, health and environmental properties of the substances. This report covers Phase II efforts.

Sixty-one substances were studied during Phase II of this project. Data on chemical and physical properties, Army and other uses, analytical methods, health effects, environmental effects, standards and regulations, and disposal methods were obtained on each substance researched.

Results of this project with respect to data gaps are presented below. Physical and chemical data; analytical methods; and health effects areas had the better data coverage. Twenty substances had insufficient direct health effects data and were characterized using structural analogues. Additional research is required for these 20 substances.

AREA	ESSENTIALLY COMPLETE	SOME GAPS	SEVERE GAPS
Physical and Chemical Data	40	15	5
Analytical Methods	43	8	9
Health Effects	35	24	1
Environmental Effects	18	26	16
Standards and Regulations	15	33	12
Disposal Methods	35	23	2

EXECUTIVE SUMMARY

The U.S. Army uses a variety of substances on a regular basis in accomplishing the missions of training, defense, and weapons development. These materials include pyrotechnics, fuels, explosives, obscurants, propellants, solvents, lubricants, preservatives, and chemical intermediates. The diversity of the substances brings about a wide range of uses, storage and disposal methods. Humans and the environment are exposed to these substances in varying amounts.

The U.S. Army Medical Bioengineering Research and Development Laboratory (USAMBRDL) was charged with identifying hazards of materials currently being used by the Army. Proper research planning required identification of the compound and, especially, informational gaps in health and environmental data. What is required, therefore, is development of a data base on health and environmental effects of waste materials generated by the U.S. Army.

This project was divided into two phases:

- o Phase I consisted of identification of Army-unique materials for inclusion in the data base.
- o Phase II consisted of researching, aggregating, and reporting data on physical, chemical, health, and environmental properties of the substances identified in Phase I and identifying data gaps.

This report covers Phase II efforts. Phase I efforts are reported in detail in a separate document prepared under this contract, "Phase I Report, May 1, 1985."

The following types of data were obtained on each substance during this study:

- o Chemical and physical data
- o Army and other uses
- o Analytical methods
- o Health effects
- o Environmental effects
- o Standards and regulations
- o Disposal methods.

Both manual and computerized methods of literature search were used. Twenty-four computerized databases were consulted.

The methodology included searching twenty-four computerized databases for physical and chemical properties. Handbooks, such as the Chemical Rubber Company Handbook of Chemistry and Physics, and Army references were used to confirm, and supplement database information. Material Safety Data Sheets and Hazardous Component Safety Data Sheets were used as alternate sources for supplementing database information.

Army Hazardous Component Safety Data Sheets and Army Technical Publications provided Army use data. Interviews with Army personnel also provided information. Civilian use information was obtained from handbooks and from databases. Army technical literature, and vendors were consulted if other sources were inadequate.

Analytical methods were obtained from databases and were evaluated using the following criterion: Trace or forensic analytical methods or those using separation were preferred. If more than one method satisfied the above criteria, both were reported. Environmental, health effects, and health related standards and regulation data were obtained from the literature, from specialized computerized databases, and by estimation. Bioconcentration factors were estimated using the Veith equation whenever possible. Whenever literature reported experimentally-determined values of bioconcentration factor, both estimated and experimental values were reported together.

Data from Section 8(e) of the Toxic Substances Control Act supplemented handbook data. Characterization of toxic effects for substances with little or no toxicity data was completed using information based on structure/activity relationships (SAR).

Environmentally related standards and regulations were obtained from the Federal Register, and from specialized databases.

Three types of disposals were considered during Phase II:

- o Current Recommended Army Disposal Practices
- o Alternate Disposal Practices under Consideration by the Army
- o Other Disposal Practices Employed.

Disposal practices were obtained from Army reports, private communications, manuals, and chemical supply catalogs.

Sixty-one substances were studied during Phase II (Exhibit II-1) of this project. Acetic anhydride was eliminated from further consideration in Phase II because rapid hydrolysis poses a minimal threat on release to the environment.

Potassium dinitrobenzofuroxan was particularly difficult to characterize because data on empirical and structural formulas were significantly different from data reported in Army references. A recent article confirming the structure through infrared and nuclear magnetic resonance spectroscopy was evaluated and incorporated. Lead styphnate had four different formulas, structures, Registry Numbers, molecular weights and index names.

Twenty substances had little or no toxicity data (Exhibit III-1). In the absence of data, toxicity information about structurally related substances or substance classes was reported. Few, if any, substances had complete environmental coverage. Physical and chemical data, analytical methods, and health areas had the better data coverage. Regulations had poor coverage, but new regulations will soon be issued covering many of the substances discussed in this report.

Data gaps in the project are listed below and in more detail in Exhibit III-2.

AREA	ESSENTIALLY COMPLETE	SOME GAPS	SEVERE GAPS
Physical and Chemical Data	40	15	5
Analytical Methods	43	8	9
Health Effects	35	25	1
Environmental Effects	18	26	16
Standards and Regulations	15	33	12
Disposal Methods	35	23	2

Based on results presented in Section III, the largest number of data gaps were found in the following areas:

- o Environmental Effects
- o Health Effects.

In no case did Environmental Effects have total data coverage, even for well-documented compounds. This lack of coverage is believed to be caused by lack of research in some specialized areas. Additional research would be required for total coverage if desired. Twenty substances had insufficient direct health effects data and were characterized by using structural analogues (Exhibit III-1). Additional research is required to conclusively identify health effects of those 20 substances.

In general, waste preservatives, inorganic obscurants and new or experimental ordnances appeared to have less data available than other substances. Almost no data were available for magnesium thorium alloy, which has fairly widespread use and possesses many apparent environmental and occupational hazards. It is recommended that research be conducted on hazards of this waste substance. While data were available on analytical method descriptions, data coverage of lower limits of detection was poor. Further research is needed to clarify this area.

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I. INTRODUCTION

A. BACKGROUND

The U.S. Army uses many substances on a regular basis in accomplishing the missions of training, defense, and weapons development. These materials include a wide range of pyrotechnics, fuels, explosives, obscurants, propellants, solvents, lubricants, preservatives, chemical intermediates, and chemical-bacteriological warfare agents.

These Army materials have a broad range of uses, storage, and disposal practices. At any time, humans may be exposed to these materials in varying amounts. The U.S. Army felt that a complete assessment of the effects of these substances on the environment and on human beings was necessary so that consistent and valid handling and disposal standards could be developed.

The U.S. Army Medical Bioengineering Research and Development Laboratory (USAMBRDL) was charged with the responsibility for developing a data base on environmental effects of waste materials generated by the U.S. Army. This data base was to include state-of-the-art knowledge about both health and environmental effects of release of these substances, chemical and physical properties, current uses (both military and civilian), methods of analysis, and current, proposed, or alternate disposal methods. This data base will be used by the Army to develop internal environmental standards for safe and effective handling of these substances.

This project was divided into two phases according to the contract. Phase I consisted of identification of Army-unique materials so that USAMBRDL could select materials to be included in the data base. Phase II consisted of researching, aggregating, and reporting data on physical, chemical, health, and environmental properties of the substances identified in Phase I and locating data gaps to be completed by additional research. This report covers Phase II. Phase I efforts are reported in detail in a separate document prepared under this contract, "Phase I Report, May 1, 1985."

B. PURPOSE

In accordance with the goals discussed above, the U.S. Army has contracted with CARLTECH ASSOCIATES, INC. to prepare a list of Army-unique compounds and to assemble a data base on these substances. This report presents both the data base and the results of efforts identified 61 chemicals in Phase I and analyzed them in Phase II.

C. ORGANIZATION

Section II of this report covers methodologies used to obtain the physical, chemical, environmental, and health data required for Phase II. Section III presents results of this research. Section IV covers conclusions and recommendations. Appendix A contains explanatory material and Appendix B contains the data base of 60 substances. Each waste substance is described in a self-contained chemical report which presents data and also includes references and other information used.

II. METHODOLOGY

A. DATA BASE AGGREGATION AND ORGANIZATION

Sixty-one waste substances were identified in Phase I (Exhibit II-1). Twenty-one waste substances were discussed in an earlier series of chemical reports prepared by the Atlantic Research Corporation (ARC) (1). Only data more recent than ARC were reported. A data form was developed to record aggregated data on each individual waste substance (Exhibit II-2).

B. CHEMICAL AND PHYSICAL DATA

1. Structure and Chemical Formulas and Molecular Weight

Structures and chemical formulas were obtained from several sources and were cross-checked whenever possible. Both the Chemical Abstract Registry File (CAS Online) and the Structure and Nomenclature Search System (SANSS), available through Information Consultants, Incorporated-Chemical Information System (ICIS) were used to supply structure and chemical formula data for all compounds. Use of these online databases is discussed in more detail in the following section. Handbooks and other references were consulted to confirm or supplement database information.

Molecular weight could not be found for a few compounds, so molecular weight was calculated, using the CAS or SANSS empirical formulas and the current International Union of Pure and Applied Chemistry (IUPAC) atomic weights for the constituent elements.

2. Alternate Names and Registry Numbers

This segment of the project identified the common or trivial name of a compound, the correct Chemical Abstracts Collective Index name(s), synonyms, CAS Registry Number, and RTECS Registry Numbers, where possible. Determination of the correct CAS registry number was the first step in preparation of a data base substance file. Obtaining subsequent data such as physical and chemical properties and health effects depended on successful completion of this step.

3. Chemical and Physical Properties

Information on sources included the following:

- o ICIS database system was searched for physical and chemical properties using CAS Registry Numbers and synonyms.
- o Oil and Hazardous Material Technical Assistance Data System (OHMTADS) was searched for reactivity, corrosivity, synergistic materials, antagonistic materials, field and laboratory detection, flammability, flash point, autoignition point, explosiveness, melting and boiling points, solubility, specific gravity, vapor pressure and vapor density.

- o ENVIROFATE, an ICIS database, supplied solubility and vapor pressure data and a few octanol/water partition coefficients.
- o Information Consultants, Inc.-Chemical Information System, Information for Hazardous Organics in Water (ICIS ISHOW), supplied octanol/water/partition coefficients. Some partition coefficients were estimated by Drs. Leo and Hantsch (7).
- o Handbooks included Chemical Rubber Company Handbook of Chemistry and Physics (2), the Merck Index (3), the Encyclopedia of Explosives and Related Items (4), the Army Engineering Design Handbook Properties of Explosives of Military Interest and the Urbanski four volume monograph on chemistry of explosives (5) (6).
- o Alternate sources were Material Safety Data Sheets and Hazardous Component Safety Data Sheets.

C. USES

Army use data were obtained from interviews with Army personnel, Army Hazardous Component Safety Data Sheets, Army Technical Publications, and literature published or sponsored by the Army in the civilian sector.

Civilian use information was obtained from the same sources listed in the chemical and physical properties section. If the compound was listed in the 1985 Chemical Buyers' Directory, the manufacturer or vendor was contacted if no other source of information was available.

D. ANALYTICAL METHODS

Analytical methods were obtained from citations retrieved by an online database search of STN International's Chemical Abstracts File, which is the computerized searchable form of the printed Chemical Abstracts. Using advanced search strategy, a query "hedge" was formulated to retrieve relevant citations from Chemical Abstracts.

Highly posted compounds such as ethylene glycol were searched by limiting the range to a particular time period which would provide the most recent information. The search on these particular compounds was limited to January, 1984 to present.

Substances not considered analytical reagents or solvents were searched using the Boolean "AND." Substance reports which were ARC updates were limited by range to January, 1984 to present since only updating was required.

Hard copies of citations were retrieved from libraries. Because many articles were inaccessible through usual retrieval methods, an extended abstract, including all bibliographic and indexing information, was retrieved from the CA file and used in this project. Search methods are discussed in more detail in Appendix A.

Analytical methods for each compound were evaluated using the following criteria:

- o Methods for trace or forensic analysis, when available, were chosen over quality control methods. Trace methods were more applicable for the evaluation of health or environmental effects. If no trace methods were published, then quality control methods were included to indicate a direction for analytical chemists to follow.
- o Preferred methods included separation or the compound-specific method. These methods are more applicable for the evaluation of health or environmental effects because the compound is usually found in complex analytical matrices such as soil, water, urine, or blood.
- o If more than one method satisfied the above criteria, both were reported because the best available method for a laboratory is one capable of using available equipment to reach the required sensitivity. However, the most sensitive method published on a given technique was chosen for discussion.
- o For inorganic salts, if no methods were available for the compound as a whole species, methods were discussed for each component part. For each method chosen, the application, the technique, the equipment required, sample type, and limit of detection were reported.

E. HEALTH EFFECTS

Collection of health effects data involved retrieval and extraction of information dealing with the toxicity of the chemicals examined.

1. Literature Retrieval

Data were obtained from computerized databases and literature listed below.

- o Chemical Hazard Information Profiles (CHIP's), Office of Pesticides and Toxic Substances, U.S. Environmental Protection Agency
- o IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans (Volumes 1-29 on Chemicals, Industrial Processes, and Industries Associated with Cancer in Humans)
- o National Cancer Institute, National Toxicology Program Technical Reports on the Toxicology and Carcinogenesis Studies of Various Chemicals
- o NIOSH Criteria Documents
- o Several health-effects handbooks were also searched on a routine basis for health data (2,3,8,9,10,11,12,13,14,15,16,17,18,19,20, 21,22,23)

- o Material safety data sheets
- o Section 8(e) of the Toxic Substances Control Act, Environmental Protection Agency
- o MEDLARS, National Library of Medicine (used for data retrieval).

The NIOSH Registry of Toxic Effects of Chemical Substances (RTECS) (22) data record was examined to determine the existence of positive data on specific chemicals. If RTECS and other handbooks contained necessary toxicity data, no further searches were conducted. TOXLINE and its two backfiles were searched for back-up data. Chemicals in the 1978 AMC updates and in the TOXBACK 1965 file (1965 to 1974) were not searched. The workscope of this project limited the number of articles or reports to six. Thus, original research reports were selected for chemicals with limited data base and manual citations. Recent review articles, when available, were selected for chemicals with more than 30 citations in the bibliographic databases.

Foreign language articles generally were not used, but English abstracts of foreign language articles were used for some chemicals with limited data. Articles and reports were obtained from Washington D.C. area libraries; Defense Technical Information Center (DTIC), Alexandria, Va; and National Technical Information Service (NTIS), Springfield, Va.

2. Structure Activity/Relationship Data

Considerable project effort was devoted to toxic effects characterization of substances with little or no toxicity data. Information based on structure/activity relationships (SAR) was obtained for these chemicals. Preliminary research was necessary to determine a feasible application of SAR data for incorporation in this report. Several SAR methods were researched (See Section III-B).

3. Data Aggregation

Data from reference books and the RTECS data base were not evaluated. Data from primary sources, i.e., original research reports, were evaluated for test results and methodology, author's conclusions, proper laboratory practices, statistical analyses, completeness of data, and applicability to the toxic effects characterization. Study inadequacies such as the lack of a test group or failure to specify the physical state of the test chemical were reported. Data were extracted and organized into a tabular format and included in the substance reports.

Abbreviations used in both environmental and health effects tables are found in Exhibit II-3.

F. ENVIRONMENTAL EFFECTS

Environmental data were obtained from the literature and by estimation. Potential literature citations were located using environmentally oriented computerized databases which included the following:

ENVIROLINE
AQUALINE
ENVIROFATE
RTECS
OHMTADS
CHEMICAL REGULATIONS AND GUIDELINES
CHEM SEARCH
NIOSH
NTIS
ENVIRONMENTAL BIBLIOGRAPHY
GPO
POLLUTION ABSTRACTS
TSCA INITIAL INVENTORY
DTIC.

Citation titles from the databases were examined; for titles appearing promising, journals were ordered. For titles considered doubtful, abstracts were requested and reviewed. Handbooks were also used (24). Occasionally, databases such as RTECS, ENVIROFATE and OHMTADS contained directly related data. If the data appeared consistent with that found on the literature, then the information was included in the report.

Bioconcentration factors were estimated using the Veith equation whenever partition coefficient data were available:

$$\text{Log BCF} = 0.76 \text{ Log } P + 0.23 \text{ (25)., where } P \text{ is the Octanol-Water Partition coefficient.}$$

Wherever literature had experimentally-determined values of bioconcentration factor; both estimated and experimental values were reported together.

G. STANDARDS AND REGULATIONS

Health-related standards and regulations were obtained principally from the Fire Protection Manual (26) and the OHMTADS, RTECS, and Occupational Safety and Health Databases.

Environmental related standards and regulations were obtained from the Federal Register, and from the ENVIROFATE, OHMTADS, and TSCA INITIAL INVENTORY computerized databases.

H. DISPOSAL

Three types of disposal were considered during Phase II:

- o Current Recommended Army Disposal Practices
- o Alternate Disposal Practices under Consideration by the Army
- o Other Disposal Practices Employed.

Current Army disposal practices are those now used by U.S. Army installations to remove waste streams containing one or more of the 61 substances identified in Phase I of this project. These were identified from Army reports (27) and from private communications with U.S. Army personnel

(28). Data on alternative disposal practices, i.e., those under consideration by the military, were obtained from USATHAMA personnel, from the U.S. Navy CHIL Manual (11), and from Army reports. Data on civilian and other disposal practices were obtained from the same sources discussed above and also from chemical supply catalogs (29). Disposal information was evaluated and prioritized in the chemical report for a substance whenever one of two conditions was achieved:

- o The substance was identified specifically by name in the reference cited; or
- o The waste substance belonged to a class of materials discussed in the reference cited. Examples of such classes included explosives, pyrotechnics and obscurants.

I. REVIEWS

Each chemical report received three sets of reviews prior to issuance of this report. The aggregated reports were reviewed by colleagues. After incorporating comments, an "outside review," was performed by scientists and engineers who had not contributed to the earlier phases of the project. After incorporating comments, the 60 chemical reports were given final review by the technical editor and the project manager.

EXHIBIT II-1

WASTE SUBSTANCES STUDIED DURING PHASE II

SUBSTANCE NAME VS. CHEMICAL ABSTRACTS SERVICE (CAS) REGISTRY NUMBER

CAS NUMBER	COMPOUND NAME	PROJECT FILE NUMBER
7446-70-0	aluminum chloride	02
2582-30-1	aminoguanidine bicarbonate	03
123-51-3	iso-amyl alcohol	04
110-46-3	iso-amyl nitrite	05
1345-04-6	antimony trisulfide	06
1304-29-6	barium peroxide	07
59744-77-3	battery lithium	08
94-36-0	benzoyl peroxide	09
9007-13-0	calcium resinate	10
1592-23-0	calcium stearate	11
16774-21-3	ceric ammonium nitrate	12
127-65-1	chloramine-T	13
10380-28-6	copper 8-quinolinolate	14
1338-02-9	copper naphthenate	15
108-94-1	cyclohexanone	16
106-19-4	dipropyl adipate	17
4682-03-5 87-31-0	diazodinitrophenol	18
116-52-5	dichlorodimethyl- hydantoin (DANC)	19
97-23-4	dichlorophene	20

693-21-0	diethylene glycol dinitrate	21
111-40-0	diethylene triamine	22
4096-88-2	dinitrophenyl azide (2,4-)	23
122-39-4	diphenylamine	24
85-98-3	ethyl centralite	25
107-21-1	ethylene glycol	26
628-96-6	ethylene glycol dinitrate	27
110-80-5	ethylene glycol monoethyl ether	28
75-21-8	ethylene oxide	29
80-13-7	halazone	30
302-01-2	hydrazine	31
13465-08-2	hydroxylammonium nitrate	32
13424-46-9	lead azide	33
51331-05-6 15245-44-0 12403-82-6 63918-97-8	lead styphnate	34
592-87-0	lead thiocyanate	35
12438-53-8	magnesium thorium alloy	36
2385-85-5	mirex	37
86-30-6	N-nitrosodiphenyl- amine	38
3156-73-8	nitro,2-propanol	39
119-75-5	o-nitrodiphenylamine	40
2899-02-7	octachlor carbanilide	41
100-02-7	p-nitrophenol	42

78-11-5	pentaerythritol tetranitrate	43
7719-12-2	phosphorus trichloride	44
29267-75-2	potassium dinitro- benzfuroxan	45
7778-74-7	potassium perchlorate	46
6423-43-4	propylene glycol 1,2-dinitrate	47
3457-90-7	propylene glycol 1,3-dinitrate	48
7723-14-0	phosphorus, red	49
26628-22-8	sodium azide	50
7601-89-0	sodium perchlorate anhydrous	51
814-95-9	strontium oxalate	52
28453-24-9	tetranitrocarbazole	53
479-45-8	tetryl	54
7550-45-0	titanium tetrachloride	55
67539-61-1 3058-38-6	triaminotrinitro- benzene	56
27096-29-3	triethanolammonium nitrate	57
111-22-8	triethylene glycol dinitrate	58
128-66-5	vat yellow 4	59
12185-10-3 AND 7723-14-0	white phosphorus AND phosphorus (includes all forms)	60
12001-85-3	zinc naphthenate	61

EXHIBIT II-2

CHEMICAL SUBSTANCE REPORT FORMAT

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula:

Molecular Weight:

Structural formula:

B. Alternate Names and Registry Numbers

CAS Registry Number:

Deleted Cas Registry Number:

CA Name (9CI):

CA Name (8CI):

RTECS Number:

C. Chemical and Physical Properties

Physical State:

Color:

Odor:

Melting Point:

Freezing Point:

Boiling Point:

Solubilities:

Water:

Nonaqueous Solvents:

Octanol Water Partition Coefficient:

Hygroscopicity:

Specific Gravity (Liquid):

Vapor Pressure:

Flash Point:

Specific Heat:

Heat of Combustion:

Reactivity:

Refractive Index:

Vapor Density:

Autoignition Temp:

Stability:

Flammability:

II. USES

A. Army Unique Use

B. Other Uses

III. ANALYTICAL METHODS

A. Best Acceptable Method

B. Limit of Detection

IV. HEALTH EFFECTS

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption:

A1b. Volatilization:

A1c. Infiltration:

A1d. Bioaccumulation:

A2. Transformation

A2a. Biodegradation:

A2b. Hydrolysis:

A2c. Photolysis:

A2d. Other chemical reaction:

A2e. Half-life:

B. Effects on animals

B1. Avian species:

B2. Mammalian wildlife species:

B3. Terrestrial invertebrates:

B4. Reptiles:

B5. Amphibians:

B6. Microorganisms, aquatic and soil:

B7. Aquatic species (fish and invertebrates):

Fish:

Invertebrate:

C. Effects on plants

C1. Phytotoxicity:

C2. Uptake:

C3. Metabolism:

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA:
 STEL:

B. Environmental

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

B. Alternate Disposal Practices Under Consideration by the Army

C. Other Disposal Practices

VIII. REFERENCES

EXHIBIT II-3

ABBREVIATIONS USED IN ENVIRONMENTAL AND HEALTH EFFECTS SECTIONS

Route

inh = inhalation
sc = subcutaneous
ip = intraperitoneal
iv = intravenous
im = intramuscular
occup. = occupational
exp. = exposure

NS = not specified

Effects

LD₅₀ = lowest dose expected to cause death
of 50% of an animal test population
LC₅₀ = same as LD₅₀ for inhalation studies
LD_{Lo} = lowest reported lethal dose
LC_{Lo} = same as LD_{Lo} for inhalation studies
TD_{Lo} = lowest reported toxic dose
TC_{Lo} = same as TD_{Lo} for inhalation studies

III. RESULTS

Sixty-one chemicals were studied during Phase II of this project. Acetic anhydride was not included in Phase II because it undergoes rapid hydrolysis in water to form acetic acid, a common chemical readily metabolized by most plant and animal life. Data obtained on acetic anhydride indicated that its half-life at neutral pH and normal ambient temperature (assumed to be 25°C) was less than one hour, thus not posing a significant environmental threat (31).

A. CHEMICAL AND PHYSICAL DATA

1. Structure and Chemical Formulas and Molecular Weight

Several compounds, such as calcium resinate, copper naphthenate and zinc naphthenate, do not have defined structures, formulas or molecular weights because they are salts formed from acid mixtures and are, therefore, not precisely defined.

2. Alternate Names and Registry Numbers

The Chemical Abstracts Registry File, a computerized database, lists six million compounds, each theoretically with a unique Registry Number. However, because of inherent vagueness in indexing chemical literature, compounds occasionally have more than one number. CAS makes every attempt to delete duplicate numbers, but to make a complete and comprehensive search requires identification of deleted Registry Numbers.

Two compounds, triaminotrinitrobenzene (TATB) and tetranitrocarbazole (TNC), are examples of two active registry numbers for the same compound. TNC is indexed under 9H-Carbazole, 1,3,6,8-tetranitro- and 9H-Carbazole, tetranitro-; TATB is indexed under 1,3,5-Benzenetriamine, 2,4,6-trinitro and Benzenetriamine, ar,ar,ar-trinitro-. When authors do not explicitly state the locants for the functional groups, CAS assigns citations to the general rather than the specific chemical name.

Diazodinitrophenol is listed in CAS under two completely different names. The structures appear different, but are resonance structures for the same compound. This cross-over was retrieved through the ICIS SANSS database. The Chemical Abstracts system was notified and Registry File experts agreed that this was the same compound.

White and red phosphorus posed a special problem because of identical chemical composition, but different physical properties. In addition, there were two Registry Numbers, one for phosphorus in general and one for tetrahedral phosphorus. White phosphorus is generally considered to be tetrahedral, but a search must also include the Registry Number for phosphorus. Retrieved literature must be checked to assure data are assigned to the proper allotrope.

Initial evaluation of some of the names supplied indicated insufficient information for further investigation. Octachlor carbanilide and dinitrophenyl azide existed as several geometric isomers. "Battery Lithium" did not identify a specific compound. Sodium perchlorate existed in both anhydrous and hydrated form. Further clarification was obtained from Army sources.

Additionally, dinitrophenyl azide had another problem. Searching under the compound name, dinitrophenyl azide, in ICIS' SANSS, two entries were retrieved: Benzene, 1-azido-2,4-dinitro-, RN 4096-88-2; and Hydroxylamine, O-(2-4-dinitrophenyl) RN 17508-17-1. These compounds are not the same, although they are related. Both listed the same RTECS number and synonyms, but the structures were different. In checking the CAS entries there was no cross-over of names or synonyms. The problem was eventually traced to a mechanical failure in the tape sold to ICIS by CAS and CAS was forced to recall the tape. The extent of this problem is unknown, but future searches will require both numbers to be used in databases other than CAS.

Potassium dinitrobenzofuroxan was a particularly difficult compound. The empirical and structural formulas found in CAS were significantly different from the Army references, including the Encyclopedia of Explosives and the Army Engineering Design Handbook. CARLTECH discussed with Chemical Abstracts experts the source of their information in order to explain the differences. CAS's source was an article published in France in 1969. A recent article (30), published jointly by the Naval Weapons Center at China Lake, CA and the Materials Research Laboratories of Australia, confirmed the CAS structure through infrared and nuclear magnetic resonance spectral data. The article states that the correct structure is not widely recognized in the explosives community. However, CAS also was not completely correct and the Eighth Collective Index Name was wrong and was corrected at the behest of CARLTECH.

Lead styphnate posed a different type of problem. Lead styphnate had four different formulas, structures, Registry Numbers, molecular weights, and index names. The ratio of lead to styphnate moiety varies and is sometimes undefined. Hydroxyl groups also varied. All four compounds and their Registry Numbers were included for completeness.

B. HEALTH EFFECTS

When all means of data acquisition had been exhausted, there remained 20 chemicals with little or no toxicity data (Exhibit III-1). Searches of the National Library of Medicine and citations contained in the TOXLINE data base identified work primarily in the area of drug analogues and pharmacologic receptor sites. Information obtained from an American Chemical Society Conference on SAR analysis and other sources indicated that work in the past focused on mathematical and computer modeling techniques. Environmental Protection Agency, Premanufacture Notification (PMN) submissions and other documents were examined for insight regarding the current practical application of SAR analysis. As a result of this research, the decision was that in the absence of toxicity data on the chemical of interest, toxicity data of structurally related chemicals and chemical classes would be retrieved and presented. The manual resources and automated data bases listed above were used to obtain this information.

C. ENVIRONMENTAL EFFECTS

Few substances had totally complete environmental effects descriptions. Even well-documented substances such as ethylene oxide had environmental data gaps. Clearly, the literature did not explore all environmental issues. This is discussed in more detail in section III-E.

D. DISPOSAL

A single chemical needed to be chosen for Battery Lithium, since sources listed little or no data under this heading. Lithium Dithionite is a chemical present in spent batteries. This chemical was chosen because it is most likely to be present in disposal of batteries and is most likely to be toxic in some form.

E. DATA GAPS

Data gaps identified during this project are presented in Exhibit III-2. Briefly, Exhibit III-2 shows that 40 waste substances had essentially complete information for Physical and Chemical Data. Fifteen substances had gaps in Physical and Chemical Data, and five compounds had severe gaps.

Analytical Methods showed 43 compounds had essentially complete data, eight compounds had a few gaps, and nine compounds had severe gaps. Health Effects data coverage was good, 35 compounds had essentially complete data, 24 compounds had some gaps, and one compound had severe gaps.

Environmental Effects found 18 compounds with essentially complete information and 26 waste substances with some gaps. Sixteen compounds had severe gaps in Environmental Data. Simultaneously, Standards and Regulations had 15 waste substances with essentially complete information. There were 33 substances with some gaps in information and 12 substances with severe gaps.

Disposal Methods showed 35 waste substances had essentially complete information. There were 23 compounds with some gaps in the information and two substances had severe gaps in Disposal Method data.

EXHIBIT III-1

CHEMICALS REQUIRING ANALOGUES TO PROVIDE APPROXIMATE HEALTH EFFECTS

Aminoguanidine bicarbonate

Calcium resinate

Ceric ammonium nitrate

Chloramine T

Copper 8-quinolinolate

Diazodinitrophenol

1,3-Dichloro-5,5-dimethyl
hydantoin

Dinitrophenyl azide

Halazone

Hydroxyl ammonium nitrate

Lead azide

Lead styphnate

Lithium dithionite

Magnesium thorium alloy

1-Nitro-2-propanol

Octachlor carbonyl chloride

Potassium dinitrobenzofuroxan

Strontium oxalate

Tetranitrocarbazole

Triethanol ammonium nitrate

EXHIBIT III-2
DATA GAPS IDENTIFIED
PHYSICAL & CHEMICAL DATA

ESSENTIALLY COMPLETE

Aluminum Chloride
Aminoguanidine
Bicarbonate
Iso-Amyl Alcohol
Iso-Amyl Nitrite
Antimony Trisulfide
Barium Peroxide
Battery Lithium
Benzoyl Peroxide
Calcium Resinate
Copper 8-Quinolinolate
Copper Naphthenate
Cyclohexanone
Diazodinitrophenol
Dischlorodimethyl-
hydantoin
Diethylene Glycol
Dinitrate
Diethylene Triamine-
Diphenylamine
Ethyl Centralite
Ethylene Glycol
Ethylene Glycol
Dinitrate
Ethylene Glycol
Monoethyl Ether
Ethylene Oxide
Lead Azide
Lead Styphnate
Lead Thiocyanate
Mirex
p-Nitrophenol
Pentaerythritol
Tetranitrate
Phosphorus Trichloride
Potassium
Dinitrobenzfuroxan
Potassium Perchlorate
Red Phosphorus
Sodium Azide
Sodium Perchlorate
Strontium Oxalate
Tetryl
Titanium Tetrachloride
Triaminotrinitrobenzene
Triethylene Glycol
Dinitrate
White Phosphorus

SOME GAPS

Calcium Stearate
Ceric Ammonium Nitrate
Chloramine t
di-n-Propyl Adipate
Dichlorophene
Halazone
Hydrazine
Hydroxyl Ammonium
Nitrate
n-Nitrosodiphenylamine
Nitrodiphenylamine
1,2 Propylene Glycol
Dinitrate
1,3 Propylene Glycol
Dinitrate
Tetranitrocarbazole
Vat Yellow
Zinc Naphthenate

SEVERE GAPS

Dinitrophenyl
Azide
Magnesium Thorium
Alloy
1-Nitro-2-
Propanol
Octachlor
Carbanilide
Triethanol
Ammonium Nitrate

EXHIBIT III-2 CONTINUED
DATA GAP IDENTIFIED
ANALYTICAL METHODS

ESSENTIALLY COMPLETE

Aluminum Chloride
Aminoguanidine
Bicarbonate
Iso-Amyl Alcohol
Iso-Amyl Nitrite
Antimony Trisulfide
Benzoyl Peroxide
Calcium Stearate
Chloramine t
Copper 8-Quinolinolate
Copper Naphthenate
Cyclohexanone
di-n-Propyl Adipate
Diazodinitrophenol
Dichlorophene
Diethylene Glycol
Dinitrate
Diphenylamine
Ethyl Centralite
Ethylene Glycol
Ethylene Glycol
Dinitrate
Ethylene Glycol
Monoethyl Ether
Ethylene Oxide
Halazone
Hydrazine
Hydroxyl Ammonium
Nitrate
Lead Azide
Lead Thiocyanate
Mirex
N-Nitrosodiphenylamine
Nitrodiphenylamine
p-Nitrophenol
Pentaerythritol
Tetranitrate (PETN)
Phosphorus Trichloride
Potassium Perchlorate
1,2-Propylene Glycol
Dinitrate
Red Phosphorus
Sodium Azide
Sodium Perchlorate
Tetryl
Titanium Tetrachloride
Triethanol Ammonium
Nitrate
Triethylene Glycol Dinitrate

SOME GAPS

Barium Peroxide
Calcium Resinate
Diethylene Triamine
Lead Styphnate
1,3 Propylene Glycol
Dinitrate
Strontium Oxalate
Triaminotrinitro-
benzene
Zinc Naphthenate

SEVERE GAPS

Battery Lithium
Ceric Ammonium Nitrate
Dichlorodimethyl-
hydantoin
Dinitrophenyl Azide
Magnesium Thorium Alloy
1-Nitro-2-Propanol
Octachlor Carbanilide
Potassium
Dinitrobenzfuroxan
Tetranitrocarbazole

Vat Yellow 4
White Phosphorus

EXHIBIT III-2 CONTINUED
DATA GAPS IDENTIFIED
HEALTH EFFECTS

ESSENTIALLY COMPLETE

Aluminum Chloride
Iso-Amyl Alcohol
Iso-Amyl Nitrite
Antimony Trisulfide
Barium Peroxide
Benzoyl Peroxide
Calcium Stearate
Copper Naphthenate
Cyclohexanone
Dichlorophene
Diethylene Glycol
Dinitrate
Diethylene Triamine
Diphenylamine
Ethylene Glycol
Ethylene Glycol
Dinitrate
Ethylene Glycol
Monoethyl Ether
Ethylene Oxide
Hydrazine
Mirex
N-Nitrosodiphenylamine
p-Nitrophenol
Pentaerythritol
Tetranitrate (PETN)
Phosphorus Trichloride

SOME GAPS

Aminoguanidine Bicarbonate
Battery Lithium
Calcium Resinate
Ceric Ammonium Nitrate
Chloramine-t
Copper 8-quinolinolate
Diazondinitrophenol
1,3-Dichloro-5,5-dimethylhydantoin
Di-n-propyl Adipate
Dinitrophenyl Azide
Halazone
Hydroxyl ammonium nitrate
Lead azide
Lead styphnate
Lead thiocyanate
Lithium dithionite
1-nitro-2-propanol
Octachlor carbanilide
Potassium dinitrobenzfuroxan
1,3-Propylene glycol dinitrate
Strontium oxalate
Tetranitrocarbazole
Triaminotrinitrobenzene
Triethanol ammonium nitrate

SEVERE GAPS

Magnesium Thorium
Alloy

EXHIBIT III-2 CONTINUED
DATA GAPS IDENTIFIED
HEALTH EFFECTS CONTINUED

ESSENTIALLY COMPLETE

SOME GAPS

SEVERE GAPS

Potassium Perchlorate
1,2-Propylene Glycol
Dinitrate
Red Phosphorus
Sodium Azide
Sodium Perchlorate
Tetryl
Titanium Tetrachloride
Triethylene Glycol Dinitrate
Vat Yellow 4
White Phosphorus

EXHIBIT III-2 CONTINUED
DATA GAPS IDENTIFIED
ENVIRONMENTAL EFFECTS

ESSENTIALLY COMPLETE

Iso-Amyl Nitrite
Chloramine t
Cyclohexanone
Dichlorophene
Diphenylamine
Ethylene Glycol
Ethylene Glycol
Monoethyl
Ether
Ethylene Oxide
Halazone
Hydrazine
Mirex
p-Nitrophenol
Pentaerythritol
Tetranitrate
Potassium
Perchlorate
Sodium Azide
Sodium
Perchlorate
Tetryl
White Phosphorus

SOME GAPS

Aluminum Chloride
Iso-Amyl Alcohol
Barium Peroxide
Battery Lithium
Calcium Resinate
Copper
8-Quinolinate
Copper Naphthenate
di-n-Propyl Adipate
Diethylene Triamine
Ethyl Centralite
Ethylene Glycol
Dinitrate
Hydroxyl Ammonium
Nitrate
Lead Azide
Lead Styphnate
Lead Thiocyanate
Magnesium Thorium
Alloy
n-Nitrosodiphenyl-
amine
Nitrodiphenyl-
amine
Phosphorus
Trichloride
1,3 Propylene Glycol
Dinitrate
Red Phosphorus
Strontium Oxalate
Tetranitrocarbazole
Titanium Tetrachloride
Triethylene Glycol
Dinitrate
Vat Yellow 4

SEVERE GAPS

Aminoguanidine
Bicarbonate
Antimony
Trisulfide
Benzoyl Peroxide
Calcium Stearate
Ceric Ammonium
Nitrate
Diazodinitrophenol
Dischlorodimethyl-
hydantoin
Diethylene Glycol
Dinitrate
Dinitrophenyl Azide
1-Nitro-2-Propanol
Octachlor Carbanilide
Potassium Dinitro-
benzfuroxan
1,2 Propylene
Glycol Dinitrate
Triaminotrinitro-
benzene
Triethanol Ammonium
Nitrate
Zinc Naphthenate

EXHIBIT III-2 CONTINUED
DATA GAPS IDENTIFIED
STANDARDS AND REGULATIONS

ESSENTIALLY COMPLETE

Aluminum Chloride
Antimony Trisulfide
Barium Peroxide
Calcium Stearate
Cyclohexanone
Dichlorodimethyl-
hydantoin (DANC)
Diphenylamine
Ethylene Glycol
Dinitrate
Ethylene Glycol
Monoethyl Ether
Hydrazine
Lead Azide
Lead Styphnate
Lead Thiocyanate
Red Phosphorus
White Phosphorus

SOME GAPS

Aminoguanidine
Bicarbonate
Iso-Amyl Nitrite
Battery Lithium
Benzoyl Peroxide
Calcium Resinate
Chloramine t
Copper
8-Quinolinolate
Copper Naphthenate
Di-n-Propyl
Adipate
Diazodinitro-
phenol
Dichlorophene
Diethylene Glycol
Dinitrate
Diethylene Triamine
Ethyl Centralite
Ethylene Glycol
Ethylene Oxide
Halazone
Hydroxyl Ammonium
Nitrate
Mirex
n-Nitrosodi-
phenylamine
Octachlor
Carbanilide
p-Nitrophenol
Pentaerythritol
Tetranitrate
Phosphorus
Trichloride
Potassium
Perchlorate
1,2 Propylene
Glycol Dinitrate
Sodium Azide
Sodium Perchlorate
Strontium Oxalate
Tetryl
Triethylene
Glycol Dinitrate
Vat Yellow 4
Zinc Naphthenate

SEVERE GAPS

Iso-Amyl Alcohol
Ceric Ammonium Nitrate
Dinitrophenyl Azide
Magnesium Thorium Alloy
1-Nitro-2-Propanol
Nitrodiphenylamine
Potassium
Dinitrobenzfuroxan
1,3 Propylene Glycol
Dinitrate
Tetranitrocarbazole
Titanium
Tetrachloride
Triaminotrinitro-
benzene
Triethanol Ammonium

EXHIBIT III-2 CONTINUED
DATA GAPS IDENTIFIED
DISPOSAL

ESSENTIALLY COMPLETE

Aluminum Chloride
Aminoguanidine
Bicarbonate
Barium Peroxide
Battery Lithium
Benzoyl Peroxide
Calcium Resinate
Calcium Stearate
Copper
8-Quinolinolate
Copper Naphthenate
Cyclohexanone
Dichlorodimethyl-
hydantoin (DANC)
Dichlorophene
Diethylene Glycol
Dinitrate
Diphenylamine
Ethylene Glycol
Ethylene Glycol
Dinitrate
Ethylene Oxide
Halazone
Hydrazine
Hydroxyl Ammonium
Nitrate
Lead Azide
Lead Styphnate
Mirex
Nitrodiphenylamine
p-Nitrophenol
Pentaerythritol
Tetranitrate (PETN)
Phosphorus
Trichloride
Potassium Perchlorate
Red Phosphorus
Sodium Azide
Sodium Perchlorate
Tetranitrocarbazole (TNC)
Tetryl
Titanium Tetrachloride
- White Phosphorus

SOME GAPS

Iso-Amyl Alcohol
Iso-Amyl Nitrite
Ceric Ammonium
Nitrate
Chloramine t
di-n-Propyl Adipate
Diazodinitrophenol
Diethylene Triamine
Dinitrophenyl Azide
Ethyl Centralite
Ethylene Glycol
Monoethyl Ether
Lead Thiocyanate
n-Nitrosodiphenyl-
amine
1-Nitro-2-Propanol
Octachlor Carbanilide
Potassium
Dinitrobenzfuroxan
1,2-Propylene Glycol
Dinitrate
1,3-Propylene Glycol
Dinitrate
Strontium Oxalate
Triaminotrinitro-
benzene
Triethanol Ammonium
Nitrate
Triethylene Glycol
Dinitrate
Vat Yellow 4
Zinc Naphthenate

SEVERE GAPS

Antimony Trisulfide
Magnesium Thorium Alloy

IV. CONCLUSIONS AND RECOMMENDATIONS

Based on results presented in Section III, the largest number of data gaps were found in the following areas:

- o Environmental Effects
- o Disposal Technology.
- o In no case did Environmental Effects have total data coverage even for well-documented compounds such as ethylene oxide. The lack of coverage is believed to be caused by a lack of research in specialized areas. Additional research would be required should total coverage be desired.
- o Twenty substances had insufficient direct health effects data and were characterized using structural analogues (Exhibit III-1). Additional research is required for these 20 substances to identify health effects.

In general, waste preservatives, inorganic obscuring agents, and new or experimental ordnance appeared to have less data available than other substances.

Magnesium thorium alloy, while in fairly widespread use and possessing many apparent environmental and occupational hazards, had almost no data available. It is recommended that research be performed on hazards of this waste substance.

While data were available on analytical method descriptions, data coverage of lower limits of detection was poor. Further research is needed to clarify this area.

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APPENDIX A

ANALYTICAL SEARCH METHODOLOGY

Analytical methods were obtained from citations retrieved by an online search of STN International's Chemical Abstracts File, which is the computerized searchable form of the printed Chemical Abstracts.

Using advanced search strategy, a query "hedge" (i.e., a reusable set of search terms which builds a search profile for specific topics) was formulated to retrieve relevant citations from Chemical Abstracts. The query used to search for analytical methods is as follows:

"QUE (ANAL OR ANALY? OR DETERMIN? OR DET# OR ASSAY OR MONITOR?
OR DETECT? OR QUANT? OR MICROANAL? OR MICRODET? OR CHROMATOG?
OR IDENTIF?)."

The "OR" is a Boolean "OR" instructs the computer to retrieve references indexed with either term. The "?" is the indefinite truncation symbol instructing the computer to retrieve references beginning with the stem. The "?" represents zero, one, or more letters. For example, "ANALY?" instructs the computer to retrieve analysis, analyze, analytical, etc. Indefinite truncation symbols are used only at the end of a term. The "#" is the definite internal truncation symbol instructing the computer to retrieve any references with that stem, except for one letter. For example, "SULF#TE" would result in the retrievals of sulfates and sulfites. In the above example, the internal truncation symbol was used at the end to require only one character be present, not zero or more. "DET#" was used to retrieve the various abbreviations used for determination such as detn., detm., or detr.

This query was linked with the CAS Registry Number(s) of a compound by either a Boolean "AND" or, in special cases, the "L" proximity operator. The Boolean "AND" instructs the computer to retrieve all citations where both search terms appear in the same record. This operator can be used to search the entire file or a previously retrieved answer set to include an additional term. The terms do not have to appear in the same indexing term like the title, but anywhere in the same citation record.

The "L" proximity operator was used in cases such as ethylene glycol or cyclohexanone. "L" instructs the computer to retrieve only those references where the Registry Number and a query term appeared in the same indexing term. It cannot be used in searching an answer set, but must be used in the CA file. For example, the "L" operator would retrieve an article on the detection of ethylene glycol in workplace air, but would not retrieve an article on ethylene glycol used as a solvent in the analysis of another compound, which would have been retrieved using "AND".

There are, however, two disadvantages to using this method: (1) STN limits the number of postings in an answer set; and (2) the search is very slow. This creates problems because both the analytical terms and the particular compounds are highly posted; the search exceeds the limit before completion and aborts. There are two ways to solve this problem: (1) use "AND" instead of "L." Search only the answer set created by the analytical

query "hedge" (which gives too many false hits); or (2) limit the range to a particular time period. The time limited query was preferred since this project required updating the data base with only the most recent information. The search on these particular compounds was limited to January, 1984 to present, which retrieved and abstracted articles published since 1983.

The Boolean "AND" gave quicker results with compounds which were not analytical reagents or solvents. Also, ARC update compounds were limited by range to January, 1984 to present because the basic information only required updating.

Citations identified from the above searches were retrieved from libraries. Many articles were inaccessible through usual retrieval methods. In that case, the extended abstract, including all bibliographic and indexing information, was retrieved from the CA file.

APPENDIX B. Database
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Benzoyl Peroxide	9-1
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Calcium Stearate	11-1
Ceric Ammonium Nitrate	12-1
Chloramine-T	13-1
Copper-8-Quinolinolate	14-1
Copper Naphthenate	15-1
Cyclohexanone	16-1
Di-n-Propyl Adipate	17-1
Diazodinitrophenol	18-1
Dichlorodimethylhydantoin	19-1
Dichlorophene	20-1
Diethylene Glycol Dinitrate (DEGN)	21-1
Diethylene Triamine	22-1
Dinitrophenyl Azide	23-1
Diphenylamine	24-1
Ethyl Centralite	25-1
Ethylene Glycol	26-1

Ethylene Glycol Dinitrate	27-1
Ethylene Glycol Monoethyl Ether	28-1
Ethylene Oxide	29-1
Halazone	30-1
Hydrazine	31-1
Hydroxyl Ammonium Nitrate	32-1
Lead Azide	33-1
Lead Styphnate	34-1
Lead Thiocyanate	35-1
Magnesium Thorium Alloy	36-1
Mirex	37-1
N-Nitrosodiphenylamine	38-1
1-Nitro-2-Propanol	39-1
2-Nitrodiphenylamine	40-1
Octachlor Carbanilide	41-1
p-Nitrophenol	42-1
Pentaerythritol Tetranitrate	43-1
Phosphorus Trichloride	44-1
Potassium Dinitrobenzfuroxan	45-1
Potassium Perchlorate	46-1
Propylene Glycol 1,2-Dinitrate	47-1
Propylene Glycol 1,3-Dinitrate	48-1
Red Phosphorus	49-1
Sodium Azide	50-1
Sodium Perchlorate	51-2
Strontium Oxalate	52-1
Tetranitrocarbazole	53-1
Tetryl	54-1

Titanium Tetrachloride	55-1
Triaminotrinitrobenzene	56-1
Triethanol Ammonium Nitrate	57-1
Triethylene Glycol Dinitrate	58-1
Vat Yellow 4	59-1
White Phosphorus	60-3

ACETIC ANHYDRIDE

Chemical No. 1, Acetic Anhydride, was eliminated from further consideration after being found a minimal environmental threat. Acetic anhydride was not included in Phase II because it undergoes rapid hydrolysis in water to form acetic acid, a common chemical readily metabolized by most plant and animal life. Data obtained on acetic anhydride indicated that its half-life at neutral pH and normal ambient temperature (assumed to be 25°C) was less than one hour, thus not posing a significant environmental threat (31).

ALUMINUM CHLORIDE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: AlCl_3

Molecular Weight: 133.34 (1)

Structural Formula: See exhibit 2-1

B. Alternate Names and Registry Numbers

CAS Registry Number: 7446-70-0

Deleted CAS Registry Number: 41630-01-7

CA Name (9CI): Aluminum chloride (AlCl_3)

CA Name (8CI): Aluminum chloride

RTECS Number: BD0525000

Other significant synonyms: Aluminum trichloride

C. Chemical and Physical Properties

Physical State: Hexagonal crystals (2)

Color: White (pure); gray or yellow to greenish (1)

Odor: Odor of hydrogen chloride (1)

Melting Point: 190°C at 2.5 atmospheres (2)

Boiling Point: 177.8°C , sublimes (2)

Solubilities:

Water: Combines with water with explosive violence and liberation of much heat (1); 69.9 g per 100 mL cold water at 15°C (2)

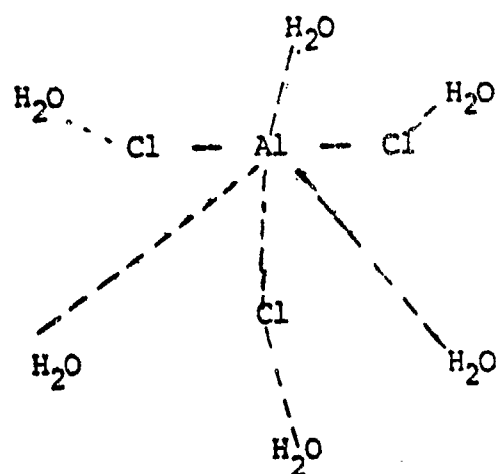
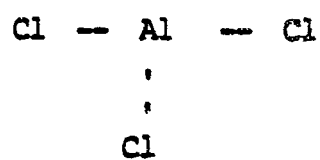
Nonaqueous Solvents: Freely soluble in many organic solvents, such as benzophenone, benzene, nitrobenzene, carbon tetrachloride, and chloroform (1); 100 g/100mL in absolute alcohol at 12.5°C ; 0.072 in chloroform at 25°C ; soluble in ether, chloroform; slightly soluble in benzene (2).

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Deliquescent (2)

ALUMINUM CHLORIDE (cont.)

EXHIBIT 2-1



ALUMINUM CHLORIDE (cont.)

Density (Crystal): 2.44 g/cc at 25 °C (2)

Specific Gravity (Liquid): 1.31 at 200 °C (2)

Volatility: Fumes in air. Volatilizes without melting when heated in small quantities (1).

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Reacts violently with water (1,2)

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Smokes and obscurants

B. Other Uses

Acid catalyst, especially in Friedel-Crafts type reactions; in cracking of petroleum; and in the manufacture of rubbers and lubricants (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

A thin-layer chromatography method has been reported for aluminum chloride and other components of water gel explosives. This method can separate and determine the various components in these mixtures. This would be the method of choice for analysis of this compound when it is found in an explosive mixture (3).

B. Limit of Detection

Data not available

ALUMINUM CHLORIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ALUMINUM CHLORIDE

Species	Route	Dose/Duration	Effects	Reference
Human	oral	0.5-5 g/kg	Estimated lethal dose	(4)
Human	contact dust	NS*	Irritating to eyes, nose and throat	(5)
Human	contact with solid	NS	Will produce skin, eye, and mouth burns	(5)
NS	NS	NS	May cause allergic reactions	(4)
Rat	oral	3.7 g/kg	LD ₅₀	(6)
Rat	NS	Acute	Increased blood glucose; decreased liver gly- cogen	(7)
Mouse	oral	770 mg/kg	LD ₅₀	(8)
Mouse	oral	425 mg/kg; multigenera- tion study	Effects on newborn	(8)
Mouse	ip	100 mmol/L	Chromosomal aberrations	(8)

* Not specified

ALUMINUM CHLORIDE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Infiltration -- Data not available

A1d. Bioaccumulation -- In Carp (Cyprinus carpio L.) exposed to 8 ppm aluminum chloride for 48 hours, concentration of aluminum in the gills exceeded 60,000 ug/g. In viscera and other parts of the fish, the aluminum concentration was less than 8,000 ug/g (9).

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

B7. Aquatic species, fish and invertebrates -- In Carp (Cyprinus carpio L.) exposed to 8 ppm aluminum chloride for 48 hours, concentration of aluminum in the gills exceeded 60,000 ug/g. In viscera and other parts of the fish, the aluminum concentration was less than 8,000 ug/g (9).

ALUMINUM CHLORIDE (cont.)

C. Effects on plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

3

TLV: TWA 2 mg(Al)/m³ (8).

B. Environmental

Reported in EPA TSCA Inventory 1980 (8).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

A recent programmatic life cycle environmental assessment indicates that incineration is the preferred method for disposal of smoke/obscurant munitions (3). Munitions containing aluminum chloride should be incinerated in a unit equipped with afterburner and a scrubber; scrubber overflow should be neutralized prior to discharge.

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

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AMINO GUANIDINE CARBONATE

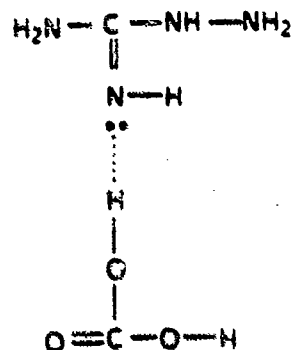
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{CH}_6\text{N}_4 \cdot \text{CH}_2\text{O}_3$

Molecular weight: 136.1

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 2582-30-1

CA Name (9CI): Carbonic acid, compound with hydrazinecarboximidamide, hydrazinecarboximidamide, carbonate

CA Name (8CI): Guanidine, amino-, carbonate, carbonic acid compound with aminoguanidine

RTECS Number: Not available in RTECS

Other Significant Synonyms: Aminoguanidine bicarbonate

C. Chemical and Physical Properties

Physical State: Solid, powder (1)

Color: White or light yellow (1)

Odor: Odorless (1)

Melting Point: 170 - 172°C with decomposition (1)

AMINOGUANIDINE CARBONATE (cont.)

Solubilities:

Water: 0.3% at 30°C; 0.2% at 20°C

Nonaqueous Solvents: Data not available

Density (Crystal): 1.47 g/cc (1)

Volatility: Not applicable

Vapor Pressure: Not applicable

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: No incompatibility (1)

Stability: Stable (1)

Flammability: No unusual fire or explosion hazards (1)

II. USES

A. Army Unique Use

Used in the manufacture of the explosive tetracene (2)

B. Other Uses

Chemical Intermediate

III. ANALYTICAL METHODS

A. Best Acceptable Method

Tanabe et al. (3) proposed a colorimetric method for guanidine and monosubstituted guanidines. The compounds were reacted with 0.04% 9,10-phenanthroquinone in dioxane:ethanol(1:4) and 2% 3,5-dihydroxybenzoic acid in ethanol and 2N potassium hydroxide; the absorbance was measured at 615 nm. This method did not include any separation from other compounds.

B. Limit of Detection

Tanabe et al. (3) claimed 0.3 to 2 micrograms.

AMINO GUANIDINE CARBONATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF AMINO GUANIDINE CARBONATE

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Aminoguanidine bi-carbonate	Rat	oral (feed)	15 mg/g	Death in 3-4 days	(4)
	Rat	oral	20 mg/kg	Specific diamine oxidase inhibitor; increased urinary excretion levels of histamine and tele-methylhistamine after histamine ingestion	(5)
Aminoguanidine	Rat	subcutaneous	1,258 mg/kg	LD ₅₀	(6)
	Rat	intravenous	7.8 mm	50% inhibition of histidine decarboxylase activity by muscular stomach homogenate or partially purified enzyme preparation from stomach muscle	(7)
	Mouse	subcutaneous	963 mg/kg	LD ₅₀	(6)
	Guinea pig	intravenous	1.7 mM	50% inhibition of activity of histamine methyltransferase isolated from brain	(7)
	Cat	intravenous	7.4-74 mg/kg	Augmented cholinergic-induced salivary excretion	(7)
	Human	subcutaneous	1 mg/kg	Abolished heparin-induced inhibition of gastric secretion; 90-95% of plasma diamine oxidase activity was inhibited	(8)
Aminoguanidine sulfate	Rat	oral	500 mg/kg	LD ₅₀	(7)

AMINO GUANIDINE CARBONATE (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of aminoguanidine bicarbonate.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Listed in EPA TSCA Inventory.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (9).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savannah Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (10).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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AMINO GUANIDINE CARBONATE (cont.)

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ISO-AMYL ALCOHOL

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_5H_{12}O$

Molecular Weight: 88.15 (1)

Structural Formula: $(CH_3)_2CHCH_2CH_2OH$

B. Alternate Names and Registry Numbers

CAS Registry Number: 123-51-3

CA Name (9CI): 1-butanol,3-methyl

CA Name (8CI): Isopentyl alcohol

RTECS Number: LV5600000, EL5425000

Other Significant Synonyms: Isobutyl carbinol (1); amyl alcohol

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Clear, oily (2)

Odor: Disagreeable, pungent, repulsive, poisonous vapors (1)

Melting Point: $-117.2^{\circ}C$ (1)

Boiling Point: $28.5^{\circ}C$ (2)

Solubilities:

Water: 2g/100 mL at $14^{\circ}C$

Nonaqueous Solvents: Miscible with alcohol, ether, benzene, chloroform, petroleum ether, glacial acetic acid, oils (1); very soluble in acetone (2); soluble in most organic solvents (2).

Partition Coefficient: $\log P = 0.46$

Hygroscopicity: Data not available

Specific gravity: 0.813 at $15^{\circ}C$

Volatility: Volatile

Vapor Pressure: 28 mm Hg at $20^{\circ}C$ (2)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Can react vigorously with reducing materials (2).

Stability: Explodes when exposed to flame (2).

Flammability: Flash point, closed cup 45°C; open cup 55°C (1)

II. USES

A. Army Unique Use

Preparation of isoamyl nitrite explosive

B. Other Uses

Solvent for fats, resins, alkaloids, etc.; manufacture of isoamyl compounds, isovaleric acid, mercury fulminate, pyroxylin, artificial silk, lacquers, and smokeless powders; in microscopy; for dehydrating celloidin solutions; and for determining fat in milk (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Gas chromatography is the method of choice. Krull et al. (3) reported an extremely sensitive method using a photoionization detector to detect the pentafluorophenyldimethylsilyl chloride (flophemsyl) derivative. Isoamyl alcohol was chromatographed on a PermaBond PEG column with temperature programming. An electron capture detector (ECD) was also used.

Masuda et al. (4) reported a gas chromatographic method for underivatized iso-amyl alcohol on a 5% phenylmethyl silicone capillary column with a flame ionization detector (FID).

B. Limit of Detection

Krull et al. (3) reported 38.7 picograms for PID and 20 picograms for ECD for the flophemsyl derivatives and 0.852 nanograms for PID and 3.37 nanograms for ECD for the underivatized alcohol.

Masuda et al. (4), 0.5mg/L or 500 ppb.

ISO-AMYL ALCOHOL (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ISO-AMYL ALCOHOL

Species	Route	Dose/Duration	Effects	Reference
Human	local	NS	Irritant; vapors rapidly produce intense irritation of nose, eyes, and throat	(5)
Human	NS	High conc.	May cause central nervous system depression, narcosis, headache, and nausea	(5)
Rat	oral	1,300 mg/kg	LD ₅₀	(6)
Rat	oral	27 g/kg (total dose), intermittently for 75 wk	Carcinogenic, producing liver and blood tumors**	(6)
Rat	intraperitoneal	813 mg/kg	LD _{Lo}	(6)
Rat	intraperitoneal	2.3 mmol/kg	Ataxia	(7)
Rat	subcutaneous	3,800 mg/kg (total dose)	Carcinogenic, producing liver and blood tumors** intermittently for 85 wk	(6)
Mouse	intraperitoneal	233 mg/kg	LD _{Lo}	(6)
Mouse	intravenous	234 mg/kg	LD ₅₀	(6)
Mouse	subcutaneous	7,480 mg/kg	LD _{Lo}	(6)
Mouse	inhalation	41,514 ppm	50% decrease in respiratory rate	(8)
Rabbit	oral	4,250 mg/kg	LD _{Lo}	(6)
Rabbit	intravenous	1,570 mg/kg	LD _{Lo} ; behavioral symptoms	(6)
Rabbit	skin	3,212 mg/kg	LD ₅₀	(6)

TABLE IV-1. TOXICITY OF ISO-AMYL ALCOHOL (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Rabbit	eye	20 mg/24 hr	Severe irritation	(6)
Cat	intra- venous	210 mg/kg	LD _{Lo}	(6)

** Conclusion taken from RTECS; studies were not evaluated

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF ISO-AMYL ALCOHOL

Test System	Dose	Effects	Reference
<u>Saccharomyces cerevisiae</u>	10 mmol/tube	Induction of chromosomal aberrations	(6)
<u>Escherichia coli</u> K12 infected with phage: lambda Tn9	"drop"	Negative results for stimulation of Tn9 transposition	(9)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Activated sludge BOD, 30 days acclimation, 20°C, 1-5 days observed, feed: 333 mg/L, 79% BOD removed (10).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

ISO-AMYL ALCOHOL (cont.)

A2d. Other chemical reaction -- BOD₅: 0.150, normal sewage as seed material, standard dilution techniques; 0.162, normal sewage as seed material, standard dilution techniques; COD: 77% of ThOD; ThOD: 2.740 (10).

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

B7. Aquatic species (fish and invertebrates) -- Data not available

C. Effects on plants

C1. Phytotoxicity -- Data not available

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Indication in Holston Installation Assessment that open burning is the only Army approved method for disposal of explosive wastes. Solvents containing up to 80-90% water are burned in clay lined pits at Holston (11).

B. Alternate Disposal Practices under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

AEHA: NSN 6810-00-142-8764, 106-8925, 2811999

Dispose of through a commercial contractor (12).

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ISO-AMYL ALCOHOL (cont.)

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(ISO) AMYL NITRITE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_5H_{11}NO_2$

Molecular Weight: 117.15 (1)

Structural Formula: $(CH_3)_2CHCH_2CH_2ONO$

B. Alternate Names and Registry Numbers

CAS Registry Number: 110-46-3

CA Name (9CI): Nitrous acid, 3-methylbutyl ester

CA Name (8CI): Isopentyl alcohol, nitrite

RTECS Number: NT0187500

Other Significant Synonyms: Isoamyl nitrite, isopentyl nitrite, 3-methylbutanol nitrite, 3-methylbutyl nitrite.

C. Chemical and Physical Properties

Physical State: Liquid (2); decomposes on exposure to air, light or water.

Color: Clear yellowish (2)

Odor: Fragrant odor and pungent aromatic taste (3)

Melting Point: Data not available

Boiling Point 96-99°C (2)

Solubilities:

Water: Very slightly soluble (1)

Nonaqueous Solvents: Miscible with alcohol chloroform, ether, and light petroleum (4).

Density: 0.8528 g/cc at 4°C (2)

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Vapor): 4.0 (2)

Volatility: Volatilizes readily (1)

Vapor Pressure (p): 60 Torr (30°C)

Flash Point: 10°C

Specific Heat: Data not available

Heat of Combustion: 6,930 cal/g

Autoignition Temperature: In air 209°C; in oxygen 202°C (5)

Reactivity: Oxidizing material, can react with oxidizing or reducing materials (2). Dangerous fire risk (4). Floats on water. Produces poisonous gas on contact with water. Combustion products include toxic oxides of nitrogen. Decomposes on exposure to air, light, or water; evolving toxic oxides of nitrogen (6). Incompatible with alcohol, alkaline, carbonates, caustic alkalis, bromides, iodides, ferrous salts, and phenazone (3). Forms an explosive mixture with air or oxygen (1).

Stability: Unstable, decomposes on exposure to air and light (1)

Flammability: Very flammable (1); moderate fire hazard when exposed to heat or flame or by spontaneous chemical reaction. Vapor explodes when heated (2).

II. USES

A. Army Unique Use

Explosive and chemical agent antidote.

B. Other Use

Perfumes, diazonium compounds (4), vasodilator (10), treatment of cyanide poisoning and H₂S poisoning (3).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Carignan and Hickman published a quantitative infrared spectrophotometric method for the determination of isomyl nitrite (7). Das et al. reported a chemical ionization mass spectrometry, in conjunction with gas chromatography, that can be used for quantitative estimation of trace amounts (8).

B. Limit of Detection

Data not available

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF AMYL NITRITE

Species	Route	Dose/ Duration	Effects	Reference
Human	oral or inhalation	NS*	Methemoglobinemia, tachycardia, headache, weakness, confusion, restlessness, faintness and loss of consciousness	(6)
Human	skin	(Liquid)	Severe skin irritation and eye damage; second and third degree burns on short contact	(6)
Human	inhalation	Therapeutic level doses(0.18 or 0.3 mL)	Headache, dizziness, weakness, postural hypotension, skin rash, and methemoglobinemia	(9)
Rat	oral	505 mg/kg	LD ₅₀	(10)
Rat	inhalation	1,274 ppm/1hr	LC ₅₀	(10)

* Not specified

TABLE IV-2. MUTAGENICITY OF AMYL NITRITE

Test System	Dose	Effects	Reference
<u>S. typhimurium</u> (strain not stated in abstract)	NS*	Mutagenic with or with- out metabolic activation	(11)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- No potential for concentration in the food chain (6).

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Decomposes on exposure to water, evolving toxic oxides of nitrogen (6).

A2c. Photolysis -- Decomposes on exposure to light, evolving toxic oxides of nitrogen (6).

A2d. Other chemical reaction -- Decomposes on exposure to air, evolving toxic oxides of nitrogen (6).

A2e. Half-life -- Data not available

B. Effects on animals -- Data not available

C. Effects on plants -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF AMYL NITRITE

Species	Route	Dose/ Duration	Effects	Reference
Human	oral or inhalation	NS*	Methemoglobinemia, tachacardia, headache, weakness, confusion, restlessness, faintness and loss of consciousness	(6)
Human	skin	(Liquid)	Severe skin irritation and eye damage; second and third degree burns on short contact	(6)
Human	inhalation	Therapeutic level doses(0.18 or 0.3 mL)	Headache, dizziness, weakness, postural hypotension, skin rash, and methemoglobinemia	(9)
Rat	oral	505 mg/kg	LD ₅₀	(10)
Rat	inhalation	1,274 ppm/1hr	LC ₅₀	(10)

* Not specified

TABLE IV-2. MUTAGENICITY OF AMYL NITRITE

Test System	Dose	Effects	Reference
<u>S. typhimurium</u> (strain not stated in abstract)	NS*	Mutagenic with or with- out metabolic activation	(11)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- No potential for concentration in the food chain (6).

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Decomposes on exposure to water, evolving toxic oxides of nitrogen (6).

A2c. Photolysis -- Decomposes on exposure to light, evolving toxic oxides of nitrogen (6).

A2d. Other chemical reaction -- Decomposes on exposure to air, evolving toxic oxides of nitrogen (6).

A2e. Half-life -- Data not available

B. Effects on animals -- Data not available

C. Effects on plants -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been

confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (12).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot. (13)

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Windholz, M., S. Budavari, R.F. Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 738. Merck and Co., Inc. Rahway, NJ.
2. Sax, N.I. 1979. Dangerous Properties of Industrial Materials, 5th ed., p. 377. Van Nostrand-Reinhold Co., New York, NY.
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5. Fedoroff, Basil T. 1960. Encyclopedia of Explosives and Related Items, Vol. 1, p. A397. U.S. Army Armament and Research Command, Dover, NJ.
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8. Das, R.C., O. Koga, and S. Suzuki. 1979. Chemical Ionization Mass Spectrometry of Alkyl Nitrates and Nitrites. Bulletin of the Chemistry Society of Japan. p. 65-8.
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(ISC) AMYL NITRITE (cont.)

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ANTIMONY TRISULFIDE

Update of Atlantic Research Corporation Study

SUMMARY OF PREVIOUS STUDY

The toxicological and environmental hazards of antimony trisulfide have been reported in the Atlantic Research Corporation's (ARC) report, A Preliminary Problem Definition Study of the Toxicological and Environmental Hazards of 48 Munitions Related Chemicals. The report concluded that the compound is not highly toxic to mammals, aquatic organisms, microorganisms or plants. A summary of chronic inhalation toxicity of antimony trisulfide to mammals was presented and the effects of antimony exposure on workers was summarized. Antimony trisulfide occurs in nature as stibnite ore. The acute toxicity of several antimony compounds to aquatic organisms was reported in the study. Phytotoxicity information is very limited.

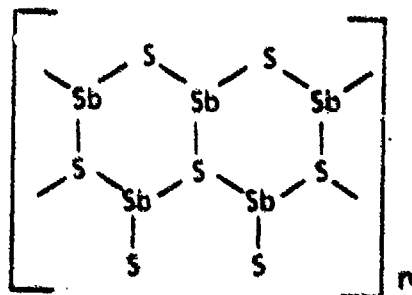
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: Sb_2S_3

Molecular Weight: 339.69

Structural Formula:



B. Alternate Names and Registry Numbers

Deleted CAS Registry Numbers: 12138-10-2; 28767-59-1

CAS Registry Number: 1345-04-6

CA Name (9CI): Antimony sulfide (Sb_2S_3)

ANTIMONY TRISULFIDE (cont.)

CA Name (8CI): Antimony sulfide

RTECS Number: CC9450000

Other Significant Synonyms: Antimony sesquisulfide, antimonous sulfide, antimony glance, antimony orange, antimony trisulfide colloid, crimson antimony sulphide, needle antimony (8).

C. Chemical and Physical Properties

Physical State: Crystals or powder (1)

Color: Gray, gray-black, orange-red to black (1)

Odor: Data not available

Melting Point: 546°C (2)

Boiling Point: 1150°C (3)

Solubilities:

Water: Insoluble (3), 0.0-0.00175 g/cc (18°C)

Nonaqueous Solvents: Soluble in alcohol, hydrochloric acid, ammonium sulfide, potassium sulfide; insoluble in acetic acid (4); soluble in sulfide salts (5); soluble in fixed alkali hydroxides (1).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): 4.64 g/cc for gray crystals and 4.12 g/cc for yellow-red solid (6).

Volatility: Data not available

Vapor Pressure: 0.033 mm Hg at 400°C; 1.17 mm Hg at 500°C; 244.00 mm Hg at 850°C (2).

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Can react vigorously with oxidizing materials and produce toxic fumes of oxides, sulfur, and antimony.

Stability: Stable in air at room temperature (2)

Flammability: Moderate fire and combustion hazard (2)

ANTIMONY TRISULFIDE (cont.)

II. USES

A. Army Unique Use

Used in pyrotechnic and primer formulations, as well as camouflage paints (2).

B. Other Uses

Used in the manufacture of vermillion or yellow pigment, antimony salts, matches, percussion caps, fireworks, and ruby glass. Also used in flame-proofing formulations (2).

III. ANALYTICAL METHODS

A. Best Acceptable Method

No analytical methods have been found by surveying the chemical literature from 1983 until present that significantly replace or update the findings in the Atlantic Research Corporation study.

B. Limit of Detection

Data not available

ANTIMONY TRISULFIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. HEALTH EFFECTS OF ANTIMONY TRISULFIDE* (7)

Compound	Species	Route	Dose/Duration	Effects
Antimony trisulfide	Human	inhalation (occup. exp.)	0.58-5.5 mg/m ³ , 8-24 mo, urinary level: 0.8-9.6 mg/L	ECG changes, cardiac deaths, ulcers
Antimony trisulfide, metal, and trioxide	Human	inhalation (occup. exp.)	urinary level: 5-182 mg/L	Female reproductive problems, infant weight gain lower than normal
Antimony trisulfide	Rat	intra-peritoneal	Single sub-lethal dose	Chronic heart changes
Antimony trisulfide or trioxide	Rat	intra-tracheal	Single 20 mg dose	Weight reduction, macrophage reaction

* Information not included in the ARC report

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of antimony trisulfide which would update the Atlantic Research Corporation study.

ANTIMONY TRISULFIDE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 0.5 mg (Sb)/m³ (8).

B. Environmental

Reported in the EPA TSCA Inventory 1983.

EPA TSCA 8(a) Preliminary Assessment Information, final rule (9).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Data not available

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data Not available

VIII. REFERENCES

1. Windholz, M., S. Budavari, R.F. Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 104. Merck and Co., Inc., Rahway, NJ.
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4. Weast, R.C. 1984-85. CRC Handbook of Chemistry and Physics, 48th ed., p. B-74. The Chemical Rubber Company, Cleveland, OH.
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ANTIMONY TRISULFIDE (cont.)

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8. Chemical Information Search (CIS), Registry of Toxic Effects of Chemical Substances (RTECS). Accession No. CC9450000. 1985.
9. Federal Register, Vol. 47, No. 82, p. 26992.

BARIUM PEROXIDE

Much of the available data on barium peroxide has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: BaO_2

Molecular Weight: 169.36

Structural Formula: $\text{Ba}^{+2} \dots (\text{O}-\text{O})^{-2}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 1304-29-6

Alternate CAS Registry Number: 16678-58-3

Deleted CAS Registry Numbers: 55346-27-5; 61233-09-8

CA Name (9CI): Barium peroxide (BaO_2)

CA Name (8CI): Barium peroxide

RTECS Number: CR0175000

Other Significant Synonyms: Barium dioxide; barium superoxide; barium oxide.

C. Chemical and Physical Properties

Physical State: White Powder

Color: White or Grayish

Odor: Odorless (1)

Melting Point: 450°C

Boiling Point: 800°C decomposes (2)

Solubilities:

Water: Slightly, decomposes on contact with water (3)

Nonaqueous Solvents: Slightly soluble in acid and soluble in acetone (4).

BARIUM PEROXIDE (cont.)

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Data not available

Density (Crystal): 4.96 g/cm³ at 20°C (Solid) (1)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Flash Point: Not flammable (1)

Heat of Combustion: Data not available

Reactivity: Can ignite spontaneously if mixed with finely divided metals. Oxidizer, will react with organics or reducing agents. Mixtures with oxidizable material are explosive and ignite easily by friction (5).

Stability: Slowly turns into BaO₂ · 8H₂O on contact with water (6). Decomposes slowly in air²(3). Reacts with dilute or strong HCl to generate hydrogen peroxide (5).

Flammability: Not flammable (5), but container may explode in fire and may cause fire on contact with combustibles or increase intensity of fire (1).

II. USES

A. Army Unique Use

As an oxidizer in igniter, tracer and propellant formulas. Imparts a green color to pyrotechnics (5).

B. Other Uses

Bleaching animal substances, vegetable fibers and straw; glass decolorizer; manufacture H₂O₂ and oxygen; dyeing and printing textiles; with powdered aluminum in welding; in cathodes; in igniter compositions. Oxidizing agent in organic synthesis.

III. ANALYTICAL METHODS

A. Best Acceptable Method

A survey of the chemical literature from 1967 on did not result in any significant change from the Atlantic Research Corporation report.

B. Limit of Detection

Data not available

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF BARIUM PEROXIDE*

Species	Route	Dose/ Duration	Effects	Reference
Human	ingestion	NS**	Excessive salivation, vomiting, colic, diarrhea, convulsive tremors, slow, hard pulse, and elevated blood pressure; hemorrhages may occur in the stomach, intestines, and kidneys; muscular paralysis may follow	(1)
Human	inhalation	NS	Irritation of mucous membranes, throat and nose	(1)
Human	topical	NS	Severe burns of eyes and skin	(1)
Mouse	subcutaneous	50 mg/kg	LD ₅₀	(7)

* Information not included in the ARC report

** Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport — Data not available

A1a. Adsorption — Data not available

A1b. Volatilization — Data not available

BARIUM PEROXIDE (cont.)

A1c. Leachability -- Leaching of barium was studied under controlled conditions similar to conditions in which barium-containing wastes are co-disposed with domestic waste in a landfill. Eighteen to 39% of the barium leached out of the material, probably mainly in the form of organic barium complexes. Leaching of barium is higher when the barium-containing salt is located below the groundwater level. Barium chloride was the salt used in the study (8).

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on Animals

B1. Avian species - Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

B7. Aquatic species, fish and invertebrates -- Data not available

C. Effects on plants

C1. Phytotoxicity -- Data not available

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

TLV-TWA 0.5 mg (Ba)/m³ (7); OSHA standard--air 0.5 mg(Ba)/m³;
DOT: oxidize.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involves open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (9).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (10).

Disposal Methods Suggested for Related Materials: Barium flouride (careful precipitation with soda ash or slaked lime). The resulting sludge should be sent to a chemical waste landfill. Barium nitrate, barium sulfide (chemical reaction with water, caustic soda, and slaked lime). The precipitated metal sludge should be landfilled. Barite barium sulfate may be recovered for reuse in drilling muds (A-57) as an alternative to disposal (11).

C. Other Disposal Practices Employed

Disposal of Laboratory or other small amounts: Cover with at least double amount of sand to soda ash 9:1 mixture. Mix completely and uniformly. While stirring, add slowly to a large beaker of sodium sulfite solution with plastic spoon. Carefully neutralize with diluted sulfuric acid. After settling, decant the sulfate solution into a sewer with sufficient water and transport the sand to a landfill site (6).

VIII. REFERENCES

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2. Sax, N.I. 1979. Dangerous Properties of Industrial Materials, 5th ed., p. 400. Van Nostrand-Reinhold Co., New York, NY.
3. Windholz, M., S. Budavari, R.F., Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 141. Merck and Co., Inc., Rahway, NJ.

BARIUM PEROXIDE (cont.)

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5. Kitchens, J.F., W.E. Harward III., D.M. Lauter, R.S. Wentzel, and R.S. Valentine. 1978. Preliminary Problem Definition Study of 48 Munitions-Related Chemicals, Vol. IV, Primer and Trace Related Chemicals-Barium Peroxide. Final Report, AD A066310. Atlantic Research Corporation, Alexandria, VA. DAMD17-77-C-7507.
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10. Forsten, I. 1980, Disposal of Hazardous Toxic Munition Waste. Proceedings of the 1980 National Conference of Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers, Durbin, NY. 440-575.
11. Sittig, Marshall. 1981. Handbook of Toxic and Hazardous Chemicals, Noyes Publication, Park Ridge, NJ.

BATTERY LITHIUM
LITHIUM DITHIONITE

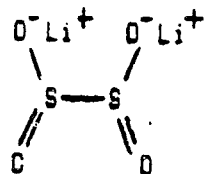
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: LiS_2O_4 (1)

Molecular Weight: 135.06 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 59744-77-3

CA Name (9CI): Dithionous acid, dilithium salt

CA Name (8CI): Data not available

RTECS Number: Not in RTECS

Other Significant Synonyms: Data not available

C. Chemical and Physical Properties

Physical State: Crystalline solid (1)

Color: White to grayish white (1)

Odor: Data not available

Melting Point: Data not available

BATTERY LITHIUM (cont.)

Solubilities:

Water: Soluble in cold water, decomposes in hot water (1)

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Is readily oxidized to bisulfite and bisulfate; when heated to decomposition in water, emits toxic vapors (1).

Stability: Data not available

Flammability: Data not available

II.

A. USES Army Unique Use

Lithium/sulfur dioxide battery; by-product formed within the lithium battery (1).

B. Other Uses

No commercial use found

III. ANALYTICAL METHODS

A. Best Acceptable Method

No method for lithium dithionite was found. Lithium could easily be detected by atomic absorption spectroscopy, but the determination would not specifically quantify the amount present as the dithionite salt.

B. Limit of Detection

Data not available

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF LITHIUM DITHIONITE

Chemical	Species	Route	Effects	Reference
Lithium dithionite			No toxicity data located on the specific compound; related data follow below	
Lithium	Human	oral	Nausea, vomiting, diarrhea, anorexia, dehydration, polyurea, apathy, lethargy, muscular weakness, ataxia, hand tremor, myoclonic twitchings, acne and exacerbation or precipitation of psoriasis, leucocytosis, headache, cogwheel rigidity; severe intoxication is associated with seriously impaired consciousness, hyperflexia, convulsions, epileptic seizures, coma, and kidney, brain, and heart damage	(2)
	Rat	NS*	Polyurea leading to oliguria and azotemia; behavioral changes begin at plasma levels of approx. 3 mmol/L; deaths above 8 mmol/L	(3)
	NS	NS	Implicated in the development of aplastic anemia	(4)
Sodium dithionite	NS	NS	Skin irritant; presumably shares the toxic potentials of bisulfite and sulfite to which it is rapidly oxidized	(5)
	Human	<u>in vitro</u>	Incubation of normal erythrocytes with sodium dithionite resulted in the formation of Heinz bodies; Heinz body formation was increased by superoxide dismutase and decreased by catalase	(6)

BATTERY LITHIUM (cont.)

TABLE IV-1. TOXICITY OF LITHIUM DITHIONITE (Cont.)

Chemical	Species	Route	Effects	Reference
Sodium bisulfite	NS	NS	Concentrated solutions are irritating to the skin and mucous membranes; in fatal poisonings, death in 30-45 min following irritability, restlessness, clonic convulsions, apnea, cyanosis, and terminal respiratory and cardiovascular collapse	(5)
	Micro-organisms	<u>in vitro</u>	Mutagenic in several test systems	(7)
Sulfites	Human	ingestion	May cause irritation of the stomach by liberating sulfurous acid	(4)
	Animals	NS	Large doses have been shown to cause retarded growth, nerve irritation, atrophy of bone marrow, depression, and paralysis	(4)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Data not available

BATTERY LITHIUM (cont.)

- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Lithium dithionite is easily oxidized to the bisulfite and the bisulfate salts in open air (8).
- A2e. Half-life -- Data not available
- B. Effects on animals
- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available
- B7. Aquatic species, fish and invertebrates -- Lithium dithionite is expected to have toxicity similar to that of other lithium salts. Lithium chloride is the best documented in Table V-1 (below)

TABLE V-1. LETHAL FISH EXPOSURES (8)

COMPOUND	ANIMAL	CONCENTRATION mg/L	EXPOSURE
Chloride	Goldfish	3750	22 to 27 Hours
Chloride	Mature Small Freshwater Fish	2600	24 Hours
Chloride	Freshwater Fish	1950-3770	24 Hours

BATTERY LITHIUM (cont.)

TABLE V-2.
LETHAL EXPOSURES OF FRESHWATER INVERTEBRATE, PROTOZOA AND BACTERIA (8)

COMPOUND	ANIMAL	PARAMETER	CONCENTRATION mg/L	EXPOSURE
Chloride	Daphnia magna	Immobilization	<7.2	----
Chloride	Daphnia magna	Poison threshold	16	48 Hours
Chloride	Scenedesmus (bact.)	No toxic effect	1000	
Chloride	E. Coli	No toxic effect	1000	
Chloride	Microregna	Food intake	66	
		Inhibition		
Chloride	Water beetle	Excitation	19500	
Chloride	Fly larvae	Toxic effect	848	

C. Effects on plants

C1. Phytotoxicity -- Concentrations of lithium ion above 30 ppm have been found to be toxic to plant species including soybeans, mustards, flax, vetch, corn, citrus, avocado and wheat (8).

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

The EPA has proposed the following limits for lithium ion in irrigation water: max 2.5 mg/L, avg 0.075 mg/L (8)

VII. DISPOSAL METHODS

A report (1) recommends secured landfills or lined disposal ponds as recommended means of lithium battery disposal.

VIII. REFERENCES

1. Crumrine, D., E. Juergens, M. Selinak, J. Fried, C. Colburn and L. McCandless. 1978. Investigation of the Environmental Consequences of Disposal of the Lithium Organic Electrolyte/SO₂ Battery. Final Report, AD A059512. U.S. Army Electronics Research and Development Command, Fort Monmouth, NJ.
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7. National Institute of Occupational Safety and Health (NIOSH). 1981-82. Registry of Toxic Effects of Chemical Substances, Vol. 3. U.S. Department of Health and Human Services, Cincinnati, OH.
8. Slimak, M., J. Freid, D. Dennedy, E. Juergens, and L. McCandless. 1977. Investigation of the Environmental Consequences of Disposal of the Lithium- Organic Electrolyte/SO₂ Battery. Phase I Report, AD A059512. U.S. Army Electronics Command, Fort Monmouth, NJ. DAAB07-76-C-1752.

BENZOYL PEROXIDE

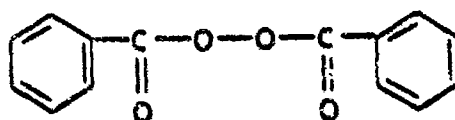
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{14}H_{10}O_4$

Molecular Weight: 242.22 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 94-36-0

Deleted CAS Registry Number: 37370-29-9

CA Name (9CI): Peroxide, dibenzoyl

CA Name (8CI): Benzoyl peroxide

RTECS Number: DM8575000

Other Significant Synonyms: Benzoyl superoxide

C. Chemical and Physical Properties

Physical State: Crystalline solid (1)

Color: White (2)

Odor: Bitter almond (2)

Melting Point: 103-106°C (1), decomposes (3)

Solubilities:

Water: Sparingly (1)

Nonaqueous Solvents: Soluble in benzene, chloroform, ether 1 g/40 mL;
carbon disulfide: . g/50 mL olive oil (1).

BENZOYL PEROXIDE (cont.)

Octanol Water Partition Coefficient: $\log P = 1.87$ (estimated)

Hygroscopicity: Data not available

Density (Crystal): 1.334 g/cc (3)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Spontaneously explodes when heated; highly reactive; sensitive to shock, heat and friction (3)

Stability: May explode when heated (1), autoignition point 68°C (3)

Flammability: Very flammable (3)

II. USES

A. Army Unique Use

Igniter formulations for explosives, pyrotechnics, and obscurants.

B. Other Uses

Oxidizer in bleaching oils, catalyst in the plastics industry, initiator in polymerization, keratolytic (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Purnell et al. (4) reported a high-performance liquid chromatography method to determine trace levels of benzoyl peroxide and other organic contaminants in workplace atmospheres. High performance liquid chromatography is used widely for quality assurance of products containing benzoyl peroxide in the pharmaceutical industry and many methods have been reported.

B. Limit of Detection

0.01 ppm (2)

BENZOYL PEROXIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF BENZOYL PEROXIDE

Species	Route	Dose/ Duration	Effects	Reference
Human	oral	0.5-5 g/kg	Estimated lethal dose	(5)
Human	local	NS*	Eye and skin irritation, skin sensitization	(5)
Human	inhalation	1.34-17.0 mg/m ³	Nose and throat irritation	(6)
Human	inhalation	2.58-82.5 mg/m ³	Eye, nose, and throat irritation	(6)
Rat	oral	7,710 mg/kg	LD ₅₀	(7)
Rat	oral	950 mg/kg	No Mortality	(5)
Rat	oral	2.8-2,800 ppm in diet for 120 wk	Testicular atrophy (not clearly chemical-related)	(6)
Rat	subcutaneous	120 mg/rat	No effects	(6)
Rat	subcutaneous implant	50 mg for 24 mo	No tumors attributed to benzoyl peroxide	(6)
Rat	inhalation	24.3 mg/L for 4 hr	Eye squint, increased and decreased respiratory rates, salivation, lacrimation, erythema; no effects after 48 hr except lingering eye irritation	(6)
Mouse	intra- peritoneal	250 mg/kg	Mortality	(5)
Mouse (hybrid hairless albino; R and CBA)	intra- peritoneal	4.8 mg/mouse	LD ₅₀	(6)

BENZOYL PEROXIDE (cont.)

TABLE IV-1. TOXICITY OF BENZOYL PEROXIDE (Cont.)

Species	Route	Dose/ Duration	Effects	Reference
Mouse	intra- pertineal	54-62 mg/kg	No effects	(6)
Mouse	subcutaneous	50 mg/mouse	No effects	(6)
Guinea pig	dermal	Dry powder	Slight irritation	(5)
Guinea pig	dermal	10% solution in propylene glycol	Slight to moderate erythema and edema without systemic toxicity	(5)
Rabbit	eye	500 mg/24 hr	Severe irritation	(7)

* Not specified

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF BENZOYL PEROXIDE

Test System	Dose	Effects	Reference
<u>Salmonella</u> <u>typhimurium</u> TA1535, TA1537, TA1538; <u>Saccharomyces</u> <u>cerevisiae</u> D4	NS*	78% benzoyl peroxide was nonmutagenic; tested with tissue homogenate from mice, rats, and monkeys for metabolic activation; benzoyl peroxide was not soluble in the vehicle DMSO	(6)
Mouse cells (type not specified)	1 μ mol/L	Mutagenic	(7)
Mouse (ICR/Ha Swiss) dominant lethal assay	54 and 62 mg/kg; ip	Negative	(6)

* Not specified

BENZOYL PEROXIDE (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of benzoyl peroxide.

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 5 mg/m³ (7)

B. Environmental

Data not available

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (8).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (9).

C. Other Disposal Practices Employed

Submerge in alkali solution 10% NaOH at 4 times weight of peroxide. Waste pastes can be charged with 50% nonflammable material (i.e., Vermiculite), dried and burned under controlled conditions. Empty containers should never be used for other purposes, but should be burned (3).

BENZOYL PEROXIDE (cont.)

VIII. REFERENCES

1. Windholz, M., S. Budavari, R.F. Blumetti, E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 159. Rahway, NJ.
2. New York State Department of Health. 1984. Chemical Fact Sheet. New York State Department of Health, Albany, NY.
3. Chemical Information System (CIS), Oil and Hazardous Materials Technical Assistance Data System (OHMTADS). Accession No. 7216603. 1985.
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5. Gosselin, Robert E., Dr., Dr. Roger P. Smith, Dr. Harold C. Hodge, and Jeannette E. Braddeck. 1984. Clinical Toxicology of Commercial Products, 5th ed. Williams and Wilkins, Baltimore, MD.
6. National Institute for Occupational Safety and Health (NIOSH). 1977. Criteria for a Recommended Standard Occupational Exposure to Benzoyl Peroxide, pp. 70-72. Department of Health, Education, and Welfare.
7. National Library of Medicine (NLM), Registry of Toxic Effects of Chemical Substances (RTECS). Accession No. DM857000. 1985.
8. David Renard, U.S. Army Toxic and Hazardous Materials Agency, to J. Carl Uhrmacher (personal communication). 1985.
9. Forsten, I. 1980. Disposal of Hazardous Toxic Munition Waste. Proceedings 1980 National Conference on Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers Division, New York. 440-375.

CALCIUM RESINATE*

*Name does not refer to a specific compound but a group of compounds, which may include the calcium salts of abietic acid, dihydroabietic acid and dehydroabietic acid (1).

*Resin acids include abietic-type acids, the pimaric-type acids and other resin acids such as elliotinoic acid (5).

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

*Chemical Formula: Not applicable

*Molecular Weight: Not applicable

*Structural Formula: See Exhibit 10-1.

B. Alternate Names and Registry Numbers

CAS Registry Number: 9007-13-0

Deleted CAS Registry Number: 68153-41-3

CA Name (9CI): Resin acids and rosin acids, calcium salts

CA Name (8CI): Same

RTECS Number: EW3970000, EW3971000

Other Significant Synonyms: Limed rosin

C. Chemical and Physical Properties

Physical State: Amorphous powder or lumps (2)

Color: Yellowish white (2)

Odor: Rosin odor (2)

Melting Point: Does not apply to mixtures

Solubilities:

Water: Insoluble (2)

Nonaqueous Solvents: Soluble in acid, amyl acetate, butyl acetate, ether, amyl alcohol (2)

Octanol Water Partition Coefficient: Not applicable

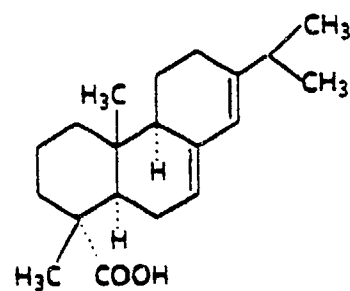
Hygroscopicity: Data not available

Density (Crystal): Data not available

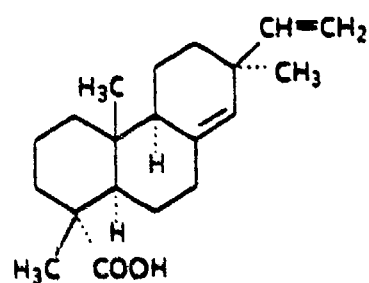
CALCIUM RESINATE (cont.)

EXHIBIT 10-1

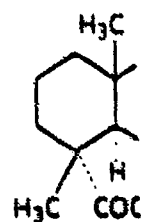
Abietic acid



Pimaric acid



Elliotinoic acid



CALCIUM RESINATE (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Can react with oxidizing materials (3)

Stability: Data not available

Flammability: Flammable, dangerous fire risk, spontaneous heating (3)

II. USES

A. Army Unique Use

Fuel, binding and water-proofing agent in primers and tracers (5).

B. Other Uses

Waterproofing, manufacture of paint driers, porcelains, perfumes, cosmetics, enamels; coatings for fabrics, wood and paper; and tanning leather (4).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Data not available

B. Limit of Detection

Data not available

CALCIUM RESINATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF CALCIUM RESINATE*

Chemical	Species	Route	Effects	Reference
Calcium resinate	NS**	ingestion	Irritation of nose and throat	(6)
	NS	topical	Contact with eyes causes irritation	(6)
	NS	NS	When rosin is heated, fumes are irritants	(11)
Resin acids:				
	NS	oral	Moderate acute toxicity	(4)
	Mouse	intravenous	LD ₅₀ : 180 mg/kg	(7)
Dehydroabiatic acid	Rat	oral	LD ₅₀ : 1,710 mg/kg	(7)

* Information not included in the ARC report

** Not specified

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of calcium resinate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

CALCIUM RESINATE (cont.)

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (8).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (9).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Windholz, M., S. Budavari, R.F. Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 1191. Merck and Co., Inc., Rahway, NJ.
2. Kitchens, J.F., W.E. Harwards III, D.M. Lauter, R.S. Wentzel, R.S. Valentine. 1978. Preliminary Problem Definition Study of 48 Munitions Related Chemicals, Vol. IV, Primer and Tracer Related Chemicals - Calcium Resinate. Atlantic Research Corporation, Alexandria, VA. DAMD17-77-C-7057.
3. National Library of Medicine, Chemical Information On-line (CHEMLINE). Accession No. 0961. 1984.
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5. Hawley, Gessner G. 1977. The Condensed Chemical Dictionary, 48th ed., p.155. Van Nostrand-Reinhold Co., New York, NY.
6. U.S. Coast Guard. 1978. Chemical Hazards Response Information System (CHRIS) Hazardous Chemical Data-Training Edition, Abridged, CG-446-2. U.S. Department of Transportation, Washington, D.C.
7. Chemical Information System (CIS), Registry of Toxic Effects of Chemical Substances (RTECS). Accession No. EW3970000. 1985.
8. David Renard, U.S. Army Toxic and Hazardous Materials Agency, to J. Carl Uhrmacher (personal communication). 1985.

CALCIUM RESINATE (cont.)

9. Forsten, I. 1980. Disposal of Hazardous Toxic Munition Waste. Proceedings of the 1980 National Conference of Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers Division, New York. 440-575.

CALCIUM STEARATE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{36}H_{70}CaO_4$

Molecular Weight: 607.00 (1)

Structural Formula: $Ca^{+2} (CH_3(CH_2)_{16}COO^{-1})_2$

B. Alternate Names and Registry Numbers

CAS Registry Number: 1592-23-0.

CA Name (9CI): Octadecanoic acid, calcium salt, stearic acid, calcium salt

RTECS Number: None

Other Significant Synonyms: Calcium distearate

C. Chemical and Physical Properties

Physical State: Granular fatty powder (1)

Color: White

Odor: Slightly fatty odor

Melting Point: 179-180°C

Solubilities:

Water: Practically insoluble (1)

Nonaqueous Solvents: Insoluble in ether, chloroform, acetone, cold alcohol. Slightly soluble in hot alcohol and hot vegetable oil.

Quite soluble in hot pyridine (1), hot ethanol, and hot mineral oil (2).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): 20 lb/ft³ (1)

Volatility: Data not available

Vapor Pressure (p): Data not available

Specific Heat: Data not available

CALCIUM STEARATE (cont.)

Heat of Combustion: Data not available

Reactivity: Decomposed by many acids and alkalies (3)

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Binder and waterproofing agent for explosive mixtures

B. Other Uses

Water repellent, paint flattening agent, lubricant in making tablets, emulsions, cements, stabilizer for vinyl resins, food additive, cosmetic ingredient (3).

Also used for waterproofing fabrics, cement, stucco; as a releasing agent for plastic molding powders; as a stabilizer for polyvinyl chloride resins; as a lubricant in pencils and wax crayons. Food grade calcium stearate, derived from edible tallow, is used as a conditioning agent in certain food and pharmaceutical products (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Hayashi et al. (4) described a high-performance liquid chromatography method using fluorescence pre-labeling with 4-(bromomethyl)-7-methoxycoumarin. The fluorescent derivatives of fatty acids were separated by reverse phase liquid chromatography followed by fluorometric detection.

B. Limit of Detection

Hayashi et al. (4) reported approximately 7 picomoles as the limit of detection in river water.

CALCIUM STEARATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF CALCIUM STEARATE

Species	Route	Dose/Duration	Effects	Reference
Rat, mouse	oral	Repeated dose, (conc. and duration NS*)	Not toxic	(5)
Rat, mouse	dermal, eye ap- plication	NS	Not toxic	(5)
Guinea pig	dermal	Emulsion (conc. NS) in egg yolk and water, daily for 14 d	Significant decrease in body weight by day 6 relative to controls	(6)
Rat	intra- tracheal	50 mg in 0.5 mL saline and 0.01 mL egg yolk; 2 or 6 mo	Severe lesions of blood vessels in pul- monary tissue at 2 mo; peribronchial sclerosis, foci of alveolar emphysema, single small areas of hemor- rhage, and pigment ag- gregations at 6 mo; results in controls not reported	(6)
Rat	intra- tracheal	10 mg in 0.5 mL saline and 0.01 mL egg yolk; 4 or 8 mo	Varying degrees of lung pathology in- cluding peribronchial sclerosis, alveolar telectasis, and dif- fuse bronchiectasis; results in controls not reported	(6)

* Not specified

V. ENVIRONMENTAL EFFECTS

No information was found on the environmental fate or effects of calcium stearate.

CALCIUM STEARATE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

The Food and Drug Administration has affirmed that calcium stearate is generally recognized as safe as a direct human food ingredient (7).

B. Environmental

Listed in TSCA inventory.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (8).

Pure or concentrated calcium stearate may not require conservative disposal methods.

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (9).

C. Other Disposal Practices Employed

Landfill in accordance with applicable local, state, and federal regulations (10).

VIII. REFERENCES

1. Windholz, M., S. Budavari, R.F. Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 234. The Merck Co., Inc., Rahway, NJ.
2. Kaye, Seymour. 1980. Encyclopedia of Explosives and Related Items, Vol. 9, PATR 2700, p. 211. U.S. Army Armament Research and Development Command, Dover, NJ.

CALCIUM STEARATE (cont.)

3. Hawley, Gessner G. 1981. The Condensed Chemical Dictionary, 10th ed., p. 186. Van Nostrand-Reinhold Co., New York, NY.
4. Hayashi, K., J. Kawase, K. Yoshimura, K. Ara, and K. Tsuji. 1984. Determination of Trace Levels of Fatty Acid and Metal Salts by High-Performance Liquid Chromatography with Fluorescence Prelabeling. Analytical Biochemistry. 136 (2):314-20.
5. Komorova, E.N. 1976. Toxic Properties of Some Additives for Plastics. Plast. Massy. 1(2):30-1.
6. Cosmetic, Toiletry, and Fragrance Association (CTFA). 1982. Final Report of the Safety Assessment of Lithium Stearate, Aluminum Distearate, Aluminum Stearate, Aluminum Tristearate, Ammonium Stearate, Calcium Stearate, Magnesium Stearate, Potassium Stearate, Sodium Stearate, and Zinc Stearate. J. Am. Coll. Toxicol. 1(2):143-77.
7. Federal Register, Vol. 48, No. 224, p. 52444.
8. David Renard, U.S. Army Toxic and Hazardous Materials Agency, to J. Carl Uhrmacher (personal communication). 1985.
9. Forsten, I. 1980. Disposal of Hazardous Toxic Munition Waste. Proceedings of 1980 National Conference on Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers Division, New York. 440-575.
10. Material Safety Data Sheet-Calcium Stearate. 1976. Diamond Shamrock Corporation, Morristown, NJ.

CERIC AMMONIUM NITRATE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{CeH}_8\text{N}_8\text{O}_{18}$ (1)

Molecular Weight: 548.26 (1)

Structural Formula: $(\text{NH}_4)_2 (\text{Ce}[\text{NO}_3]_6)$

B. Alternate Names and Registry Numbers

CAS Registry Number: 16774-21-3

Deleted CAS Registry Numbers: 25567-17-3; 15306-26-0

CA Name (9CI): Cerate(2-), hexakis(nitrato-O)-, diammonium
(OC-6-11)-

CA Name (8CI): Cerate(2-), hexanitrate-, diammonium

RTECS Number: Data not available

Other significant synonyms: Ammonium cerium nitrate; Diammonium hexanitratocerate; Ammonium hexanitratocerate; Diammonium cerium hexanitrate; Ammonium cerium hexanitrate; Ceric(IV) ammonium nitrate

C. Chemical and Physical Properties

Physical State: Crystalline solid; monoclinic (1)

Color: Orange-red (1)

Odor: Data not available

Melting Point: Data not available

Solubilities

Water: 141 g/100 mL at 25°C; 227 g/100 mL at 80°C

Nonaqueous Solvents: Soluble in alcohol, as well as nitric acid (2).

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Data not available

Density (Crystal): Data not available

CERIC AMMONIUM NITRATE (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Explosive

B. Other Uses

Catalyst for polymerization of olefin; standard in oxidimetry (1).

CERIC AMMONIUM NITRATE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

No methods of analysis for this compound have been reported in the last five years in Chemical Abstracts.

B. Limit of Detection

Data not available

CERIC AMMONIUM NITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF CERIC AMMONIUM NITRATE

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Ceric ammonium nitrate				No toxicity data located	
Nitrates	Human	oral	Large amounts	Dizziness, abdominal cramps, vomiting, bloody diarrhea, weakness, convulsions, and collapse	(3)
			Small repeated doses	May lead to weakness, general depression, headache, and mental impairment	
Cerium nitrate $\text{Ce}(\text{NO}_3)_3$	Rat	oral	3,630 mg/kg	LD_{50}	(4)
	Rat	intrates-ticular	26,092 mg/kg	TD_{10} ; effects on spermatogenesis and sex organs	(4)
Cerium nitrate hexahydrate $\text{Ce}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$	Rat	oral	4,200 mg/kg	LD_{50}	(4)
	Rat	intraperitoneal	290 mg/kg	LD_{50}	(4)
	Rat	intra-venous	4 mg/kg	LD_{50}	(4)
	Mouse	intraperitoneal	470 mg/kg	LD_{50}	(4)
Cerium salts	NS*	NS	NS	Increase in blood coagulation rate	(3)
Cerium	Human	intra-venous	3-12.5 mg/kg, single and	Anticoagulant effect for 8 hr; chills, fever, headache, muscle pains, abdomi-	(5)

CERIC AMMONIUM NITRATE (cont.)

repeated
daily
dosesnal cramps, hemoglo-
binemia, hemoglobin-
uria

* Not specified

TABLE IV-1 TOXICITY OF CERIC AMMONIUM NITRATE (Cont.)

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Cerium (cont.)	Rat	intra- venous	NS	Fatty infiltration of the liver charac- terized by an in- crease in neutral fat esters; total choles- terol and phospholipid of liver were un- changed; effects more pronounced in females	(5)
Lanthanide compound (not specified whether Ce was tested)	Rat	oral (feed)	0.01, 0.1, and 1% in diet for 12 wk	No influence on growth or hematolo- gic variables; tis- sues of 8 internal organs showed no his- tological changes at 0.01 and 0.1%; ani- mals given Gd, Tb, Tm and Yb showed non- specific liver damage (perinuclear vacuoli- zation and granular cytoplasm) at 1%	(5)

* Not specified

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects
of ceric ammonium nitrate.

CERIC AMMONIUM NITRATE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (6).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (7).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Windholz, M. S. Budavari, R.F. Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 76. Rahway, NJ.
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CHLORAMINE-T

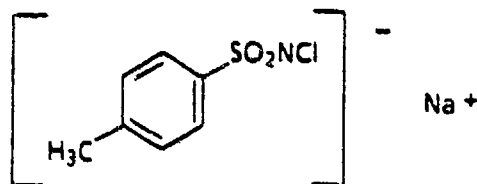
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $(C_7H_7SO_2N(Cl))Na$

Molecular Weight: 215.45

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 127-65-1

Deleted CAS Registry Numbers: 75532-46-6; 72793-59-0; 1576-40-5;
8045-11-2

CA Name (9CI): Benzenesulfonamide, N-chloro-4-methyl-, sodium salt

CA Name (8CI): p-Toluenesulfonamide, N-chloro- sodium salt

RTECS Number: 217815

Other Significant Synonyms: Sodium tosylchloramide N-Chloro-4-methylbenzyl sulfonamide, sodium salt, halamid, chlorazone

C. Chemical and Physical Properties

Physical State: Trihydrated crystal; prisms (1)

Color: White or faintly yellow (11)

Odor: Data not available

CHLORAMINE-T (cont.)

Melting Point: 167-170°C (11)

Solubilities:

Water: Fairly soluble in water (1)

Nonaqueous Solvents: Practically insoluble in benzene, chloroform, ether; decomposes in alcohol (1).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Reacts with water to release HOCl

Stability: Decomposes slowly upon exposure to air and under the influence of light (1). May decompose violently if heated above 130°C (15).

Flammability: Data not available

II. USES

A. Army Unique Use

Field water purification chemical

B. Other Uses

Antibacterial, veterinary antiseptic, laboratory detection of halogens and bromate (1).

CHLORAMINE-T (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

A titrimetric method for the determination of Chloramine-T and aldoses is based on Leipter determination of iodide by reduction with excess iodide and extraction and subsequent reduction of the iodine liberated (2).

B. Limit of Detection

0.01 mg/L (2)

CHLORAMINE-T (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF CHLORAMINE-T

Chemical	Species	Route	Effects	Reference
Chloramine-T	Human	ingestion	Vomiting, cyanosis, circulatory collapse, frothing at the mouth, and respiratory failure can occur within a few minutes, fatalities have occurred	(3)
	Human	intravenous	In tap water it has cause hemolysis in patients undergoing dialysis	(3)
	Human	inhalation	Can cause vasomotor rhinitis and asthma	(4)
	Human	occupational exposure	Nasal irritation and/or wheezing; fever; cough; asthmatic reactions	(5)
	Human	occupational exposure	Immediate asthmatic bronchial obstruction and/or a late-type asthmatic reaction accompanied by leukocytosis after inhalation tests of Chloramine-T; an immediate type of wheal and flare reaction followed by a late-type infiltrative reaction after prick tests; specific IGE antibodies occur in the sera of exposed patients	(5,6)
	Human	ingestion	An occasional reaction is rapid and violent, suggesting hypersensitivity; poisoning characterized by pain, vomiting, sudden loss of consciousness, circulatory and respiratory collapse, and death; it has been suggested that Chloramine-T can react with some amino acids in the gastrointestinal tract to form toxic cyanogen compounds	(7)

CHLORAMINE-T (cont.)

TABLE IV-1 TOXICITY OF CHLORAMINE-T (Cont.)

Chemical	Species	Route	Effects	Reference
Hypochlorous acid (available chlorine)	Human	local	Highly irritating to skin, eyes, and mucous membranes	(4)
	Human	ingestion	Irritation and corrosion of mucous membranes with pain and vomiting; a fall in blood pressure, delirium, and coma may occur	(3)
	Human	inhalation	Coughing, choking; may cause severe respiratory tract irritation and pulmonary edema	(3)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF CHLORAMINE T

Test system	Dose	Effects	Reference
<u>Salmonella typhimurium</u> (TA98, TA100, TA1535, TA1538)	4-2,500 ug/plate	Nonmutagenic with Aroclor 254-induced rat liver S9	(8)
<u>S. typhimurium</u> (TA98, TA100, TA1535, TA1537, TA1538)	several dose levels	Nonmutagenic with or without Aroclor 1254-induced rat liver S9	(9)
<u>Drosophila melanogaster</u> Basic test	25 mM; oral (approx. LD ₅₀)	No increase in frequency of sex-linked recessive lethal mutations	(9)
Micronucleus test on mouse bone marrow	35 and 70 mg/kg; ip	No increase in frequency of micronuclei	(9)
Human lymphocytes <u>in vitro</u>	100 ppm/24 hr (Chloramine-T trihydrate)	Induction of chromosomal aberrations	(10)

CHLORAMINE-T (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

- A1. Transport -- Data not available
- A1a. Adsorption -- Data not available
- A1b. Volatilization -- Data not available
- A1c. Leachability -- Data not available
- A1d. Bioaccumulation -- Data not available
- A2. Transformation -- Data not available
- A2a. Biodegradation -- Data not available
- A2b. Hydrolysis -- Releases hypochlorous acid (HOCl) in water (11)
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available

B. Effects on animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available
- B7. Aquatic species, fish and invertebrates -- After a 60-minute exposure at 25°C to 1.0 mg/L applied Chloramine-T significantly lower increases in dry weight and significant reductions in standard respiration rate were measured among exposed larval lobsters (Homarus americanus), compared to control organisms. Greater differences were detected among Chloramine-T-exposed organisms than were measured for organisms exposed to 1.0 mg/L applied free chlorine (12).

CHLORAMINE-T (cont.)

Chloramine-T was more toxic to rotifers (Brachionus plicatilis) than was the free chlorine form, with LC_{50} values for 30-minute exposures at 20 of 0.35 mg/L applied Chloramine-T and 1.20 mg/l applied free chlorine, 0.02 mg/L and 0.18 mg/L residual level, respectively. Increased temperature had a synergistic effect on the toxicity of both Chloramine-T and free chlorine. Rotifers surviving exposure to either halogen toxicant had significantly lower filtration rates and egg production rates than control animals. The reduced reproductive rates were not sustained by the second generation (13).

Shrimp (Penaeus setiferus): In a 24-hour toxicity test at a concentration of 40,000 ug/L Chloramine-T, at 21 to 22°C, 6 of 140 shrimp died (14).

Lethal concentrations: Ptychocheilus oregonensis, 0-3 hour exposure, 11.7°C: 10 ppm; Coho and Chinook salmon, 1-2.5 hour exposure, 11.7°C: 1 ppm; Rainbow trout, 1 hour exposure, 12.8°C: 5 ppm; Bluegill, 5 hour exposure, 12.8°C: 5 ppm; Pitomyzon marinus, 14 hour exposure, 12.8°C: 5 ppm (13).

C. Effects on plants

C1. Phytotoxicity -- Data not available

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Data not available

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

CHLORAMINE-T (cont.)

C. Other Disposal Practices Employed

The U.S. EPA recommends dilution in a flammable solvent followed by burning in an incinerator equipped with an afterburner and an effluent scrubber for Chloramine-T disposal. Scrubber overflow is to be neutralized prior to discharge. Incinerator ash should be buried in a hazardous or sanitary landfill (11).

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COPPER-8-QUINOLINOLATE

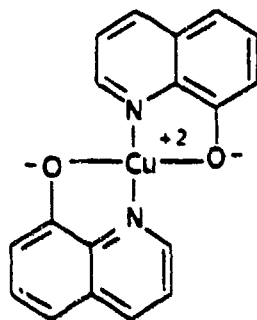
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{Cu}(\text{C}_9\text{H}_6\text{ON})_2$

Molecular Weight: 351.83

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 10380-28-6

Deleted CAS Registry Numbers: 29713-19-7; 132-71-8; 37220-44-3; 37233-52-6

CA Name (9CI): Copper, bis(8-quinolinolato-N1,08)

CA Name (8CI): Copper, bis(8-quinolinolato)-

RTECS Number: VC5250000

Other Significant Synonyms: Copper-8-quinolinolate, copper quinolate, Copper oxinate, Copper 8-hydroxyquinoline, Quinolate (1)

C. Chemical and Physical Properties

Physical State: Powder (1)

Color: Yellow-Green

Odor: Odorless

Melting Point: Decomposes at 210°C (2)

COPPER-8-QUINOLINOLATE (cont.)

Solubilities:

Water: Insoluble (1)

Nonaqueous Solvents: Somewhat soluble in weak acids, soluble in strong acids; insoluble in most organic solvents (1).

Octanol Water Partition Coefficient: $\log P = 2.70$ (3)

Hygroscopicity: Nonhygroscopic (1)

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Military anti-mildew agent

B. Other Uses

Fungicide and mildew-proofing of fabrics; reagent for the analysis of copper (1); wood preservative.

III. ANALYTICAL METHODS

A. Best Acceptable Method

No work has been done on the determination of trace amounts of this compound. 8-Quinolinoline is a strong chelating agent and may interfere with some methods of analysis of copper. Work has been done on the size exclusion (4) and thin-layer chromatographic behavior (5) of this compound. Application to trace analysis of this compound is difficult to predict. Potentiometric titration with N-bromophthalimide in aqueous acetic acid has been reported by Mohanadas and Indrasenan (6), but no method of separation was reported.

B. Limit of Detection

Data not available

COPPER-8-QUINOLINOLATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF COPPER 8-QUINOLINOLATE

Chemical	Species	Route	Effects	Reference
Copper 8-quin- olinolate	Human, Animal	NS*	Low toxicity; does not irritate the skin	(7)
Copper 8-quin- olinolate	Mouse	intra- peritoneal	LD ₅₀ : 67 mg/kg	(8)
8-Hydroxyquin- oline	Animal	NS	CNS stimulant	(2)
8-Hydroxyquin- oline	Rat	oral	LD ₅₀ : 1200 mg/kg	(2)
8-Hydroxyquin- oline	Mouse	intra- peritoneal	LD ₅₀ : 48 mg/kg	(2)
Copper salts	Human	eyes	May cause conjunctiv- itis, ulceration and turbidity of the cornea	(9)
Copper salts	Human	inhalation	May cause congestion of the nasal mucous mem- branes and pharynx, and ulceration with perfor- ation of the nasal septum	(9)
Copper salts	Human	ingestion	Salivation, nausea, vomiting, gastric pain, hemorrhagic gastritis, and diarrhea	(9)

* Not specified

COPPER-8-QUINOLINOLATE (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF COPPER 8-QUINOLINOLATE

Test System	Dose	Effects	Reference
<u>S. typhimurium</u> (TA98, TA100, TA1535, TA1537)	5 ug/plate	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(10)
<u>S. typhimurium</u> (TA100)	0.5-50 ug/ plate	Weakly mutagenic: 1.30 revertants/nmole in the presence of S9	(11)
<u>E. coli</u> (WP2 hcr)	up to 5,000 ug/plate or toxic dose	Nonmutagenic with or without S9	(11)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- 8-Hydroxyquinoline causes 75% inhibition of nitrification process in non-acclimated activated sludge at 73 mg/L (12).

B7. Aquatic species, fish and invertebrates, -- Snails: Cypangopaludina malleata: 48-hour LC₅₀: 20,000 ug/L; Semisulcospina libertina: 48-hour LC₅₀: 7700 ug/L; Indoplanorbis exustus: 48-hour LC₅₀: 15,000 ug/L; Physa acuta: 48-hour LC₅₀: 13,000 ug/L (13).C. Effects on plants

C1. Phytotoxicity -- Treatment of seeds with copper 8-quinolinolate (wet dressing with 2 cc of 15% copper 8-quinolinolate per kg of wheat seed) is effective against fungi and has a low phytotoxicity (14).

COPPER-8-QUINOLINOLATE (cont.)

- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory, 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for Copper Naphthenate, a related compound used for a related purpose, are to turn the bulk chemical into a pesticide collection center, to the original supplier or to a commercial waste disposal service (15). Data were not available on disposal of items treated with Copper Naphthenate.

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

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COPPER-8-QUINOLINOLATE (cont.)

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COPPER NAPHTHENATE

*NAPHTHENE is a term used in petroleum chemistry to denote certain saturated hydrocarbons, specifically five- and six-carbon cycloparaffins and their alkyl derivatives, found in crude petroleum. It is sometimes used to include polycyclic members found in higher-boiling fractions (1). This is not a unique chemical substance (CAS) but represents the Copper (+2) salts of naphthene carboxylic acids.

I. Chemical and Physical Data

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: Undefined

Molecular Weight: Undefined

Structural Formula: Undefined

B. Alternate Names and Registry Numbers

CAS Registry Number: 1338-02-9

CA Name: Napthenic acid, copper salt

RTECS Number: QK9100000

Other Significant Synonyms: Data not available

C. Chemical and Physical Properties

Physical State: Solid (2)

Color: Green-blue (2)

Odor: Gasoline-like (3)

Boiling Point: 154-202°C (3)

Solubilities:

Water: Insoluble

Nonaqueous Solvents: Soluble in gasoline, benzene and mineral oil distillates (4)

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

COPPER NAPHTHENATE (cont.)

Volatility: Data not available

Flash Point: 41°C

Heat of Combustion: 9,8000 cal/g (3)

Autoignition Temperature: 282°C (mineral spirit) (3)

Reactivity: Data not available

Stability: Data not available

Flammability: Flammable, moderate fire risk (2), combustible (3)

II. USES

A. Army Unique Use

Military anti-mildew agent

B. Other Uses

Wood, canvas, and rope preservative; insecticide; fungicide; antifouling paints (2)

III. ANALYTICAL METHODS

A. Best Acceptable Method

No methods were found for either copper naphthenate or naphthenic acid in searching the Chemical Abstracts System back to 1967. Copper can be analyzed by either atomic absorption spectroscopy or atomic emission spectrometry. Recently, a method was reported by Hee et al. which enhances the detection of copper by simultaneous inductively coupled plasma atomic emission spectrometry (4).

B. Limit of Detection

The lower determination range for copper is 0.001-0.005 ug/L. The apparent linear range is 2-500 ug/L (4).

COPPER NAPHTHENATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF COPPER NAPHTHENATE

Species	Route	Dose/ Duration	Effects	Reference
Human	skin	Liquid	If spilled on clothes and allowed to remain may cause smarting and redness of skin	(3)
Human	in- gestion	Liquid	Irritation to stomach	(3)
Human	inhal- ation	Liquid	Mild irritation of the respiratory tract; aspiration causes severe lung irritation and rapidly developing pulmonary edema; central nervous system excitement followed by depression	(3)
Human	eye	Liquid	Mild irritation	(3)
Rat	oral	4,000-6,000 mg/kg	LD ₅₀	(3)
Sprague-Dawley rat, 1-15 d preg	intra- peri- toneal	10,000 mg/kg *	No signs of fetal toxicity or teratogenicity	(5)
Rat, mouse	in- gestion	*	Flaccidity and narcotic effects	(6)
Mouse	oral	110 mg/kg*	LD _{Lo}	(7)

* Not specified whether the chemical was liquid or solid

COPPER NAPHTHENATE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

- A1. Transport -- Data not available
- A1a. Adsorption -- Data not available
- A1b. Volatilization -- Data not available
- A1c. Leachability -- Data not available
- A1d. Bioaccumulation -- Data not available
- A2. Transformation
- A2a. Biodegradation -- Data not available
- A2b. Hydrolysis -- Under certain conditions can hydrolyze to copper hydroxide and naphthenic acid (8).
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available

B. Effects on animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available
- B7. Aquatic species, fish and invertebrates -- Freshwater blue-green algae: 72-hour LC_{50} : 2.0 ppm (3).

C. Effects on plants

- C1. Phytotoxicity -- Burlap treated with up to 4.0% copper naphthenate was not phytotoxic to Cotoneaster divaricata when balled roots were wrapped in the burlap for 40 weeks (9).
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

COPPER NAPHTHENATE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for copper naphthenate are to turn in to a pesticide collection center, to the original supplier or to a commercial waste disposal service (10).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Adsorb on filter aid or inert powder and incinerate in approved facility, not in closed container (8).

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CYCLOHEXANONE

Update of Atlantic Research Corporation Study

SUMMARY OF PREVIOUS STUDY

It has been reported that the Army has a need for research on the toxicological and environmental hazards of cyclohexanone (4). The report states that the compound is moderately toxic in acute doses by all routes of administration. Sublethal doses cause profound narcosis accompanied by central nervous system depression. Teratogenic effects had been reported in chick embryos. There was no information on carcinogenic or mutagenic potential of cyclohexanone. The few aquatic toxicity studies available indicated a low toxicity of cyclohexanone to aquatic life.

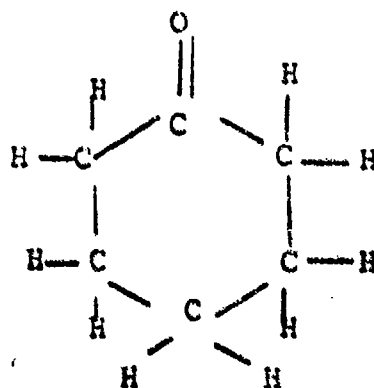
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_{10}O$

Molecular Weight: 98.14

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 108-94-1

Deleted Cas Registry Number: 48090-95-5

CA Name (9CI): Cyclohexanone

CYCLOHEXANONE (cont.)

CA Name (8CI): Cyclohexanone

RTECS Number: GW1050000

Other Significant Synonyms: Ketohexamethylene, pimelic ketone, pimelin ketone, sextone (1).

C. Chemical and Physical Properties

Physical State: Oily liquid (6)

Color: Colorless or pale yellow (6)

Odor: Peppermint and acetone (6)

Melting Point: -16.4°C

Freezing Point: -32.1°C

Boiling Point: 155.6°C at 760 mm Hg (2)

Solubilities:

Water: 50g/L at 30°C (2)

Nonaqueous Solvents: Soluble in alcohol, ether and other common organic solvents (2); acetone, benzene, chloroform (3), nitrobenzene, n-hexanone, naptha, xylene, ethylene glycol, isoamyl acetate, dimethylamine (4).

Octanol Water Partition Coefficient: $\text{Log } P = 0.81$ (5)

Hygroscopicity: Data not available

Specific Gravity (Liquid): 0.95 (18)

Vapor Pressure: 3.95 mm Hg at 20°C (4); 4.0 mm Hg at 20°C (5); 4.5 mm Hg at 20°C (5); 10 mm Hg at 38.7°C (6); 60 mm Hg at 77.5°C (6).

Flash Point: 54°C , open cup (4); 63°C (2).

Specific Heat: 0.433 cal/g at $15-18^{\circ}\text{C}$ (4)

Heat of Combustion: -8570 cal/g (4)

Reactivity: Strong oxidizers will convert cyclohexanone to adipic acid. Susceptable to nucleophilic attack (4).

Refractive Index: (N 20/D) 1.4507 (7)

Autoignition Temp: 420°C

Stability: Stable under normal conditions (4)

CYCLOHEXANONE (cont.)

Flammability: Limits (%), 1.1-8.1, moderate, flash point, 63°C, combustion with moderate heating, slight explosive hazard in vapor form when exposed to flame (6).

II. USES

A. Army Unique Use

Recrystallization solvent for RDX (4)

B. Other Uses

Organic synthesis of adipic acid and caprolactam (8). Solvent for cellulose acetate, nitrocellulose, natural resins, vinyl resins, crude rubber, waxes, fats, shellac, DDT. Also used in the production of cyclohexanone resins (2).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Recent methods developed for monitoring cyclohexanone and its methylation products in aqueous solution involve introducing the sample is introduced into a tandem mass spectrometer through semipermeable capillary tubing with a membrane interface (9). Additional methods of analysis are reported in the Atlantic Research Corporation Report. Gas chromatography is still used in the monitoring of air and water samples.

B. Limit of Detection

Detection limits are reported to be 0.0004 - 0.0005 ppm (6).

CYCLOHEXANONE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF CYCLOHEXANONE*

Species	Route	Dose/Duration	Effect	Reference
Rat	oral	1,535 mg/kg	LD ₅₀	(1)
Rat (Wistar or Gunn)	intra- venous	50 and 100 mg/kg, 1x/d for 28 d	No adverse effects on opthal- mologic, histopathologic, hematologic, or clinical chemistry parameters	(10)
Rat	subcu- taneous	2,170 mg/kg	LD ₅₀	(1)
Rat	inhalation	105 mg/m ³ /4 hr, days 1-20 of gestation	TC _{Lo} , effects on fertility	(1)
Mouse (CD-1)	oral	800 mg/kg days 8-12 of gestation	No fetotoxic effects	(11)
Mouse	subcu- taneous	1,300 mg/kg	LD _{Lo}	(1)
Mouse (Swiss OF1)	inhalation	308 ppm/4 h	50% decrease in immobility developed during a "behavioral despair" swimming test	(12)
Guinea pig	dermal	0.5 ml, 3x/wk for 3 wk	Cataracts	(13)
	subcu- taneous	0.5 ml of 5% solution in saline, 3x/wk for 3 wk	Cataracts	(13)
Dog	intra- venous	284 mg/kg/d in sodium chloride solution for 18-21 d	Signs of toxicity included: vocalization, lacrimation, scleral vasodilation, mydriasis, salivation, urination, defe- cation, restlessness, stupor and ataxia, occasional convul- sive movements, hypernea and/or dyspnea, inflammation at injec- tion site, hemolysis, bone mar- row hyperplasia, and extrane- dullary hematopoiesis	(14)

CYCLOHEXANONE (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF CYCLOHEXANONE

Test System	Dose	Effect	Reference
Human lymphocytes	5 ug/L	Mutagenic	(1)
Human leukocytes	100 umol/L	Mutagenic	(1)
<u>Salmonella</u> <u>typhimurium</u> TA98, TA100 TA1535, TA1537	3 umol/ plate	Not mutagenic with or without Aroclor 1254-induced rat liver S9	(15)
<u>S. typhimurium</u> TA98, TA100	0.03-30 umol/ plate	Not mutagenic with or without Aroclor 1254-induced rat liver S9	(15)
<u>S. typhimurium</u> TA98, TA100, TA1535, TA1537, TA1538	NS*	Mutagenic	(16)
<u>Bacillus subtilis</u>	NS	Mutagenic	(16)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Log of bioconcentration factor calculated from
octanol/water partition coefficient: log BCF = 0.56 (17).

A2. Transformation

A2a. Biodegradation -- Cyclohexanone is not biodegraded well (6).

CYCLOHEXANONE (cont.)

Biodegradation by adapted activated sludge--cyclohexanone as sole carbon source: 96.0% COD removal at 30.0 mg COD/g dry inoculum/hr (18).

- A2b. Hydrolysis -- Data not available
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- 1 BOD₅: 1.232; 32% of ThOD; COD: 100% of ThOD; ThOD: 2.605 (18).
- A2e. Half-life -- Data not available
- B. Effects on animals
 - B1. Avian species -- Data not available
 - B2. Mammalian wildlife species -- Data not available
 - B3. Terrestrial invertebrates -- Data not available
 - B4. Reptiles -- Data not available
 - B5. Amphibians -- Data not available
 - B6. Microorganisms, aquatic and soil -- Toxicity threshold by cell multiplication inhibition test: bacteria (Pseudomonas putida), 180 mg/L; algae (Microcystis aeruginosa), 52 mg/L; green algae (Scenedesmus quadricauda), 370 mg/L; protozoa (Entosiphon sulcatum), 545 mg/L; protozoa (Uronema parduzi Chatton-Lwoff), 280 mg/L (18).
 - B7. Aquatic species (fish and invertebrates) -- Fish: Leuciscus idus LC₅₀ (exposure not reported): 536000 ug/L (19); Leuciscus idus LC₅₀ (exposure not reported): 752000 ug/L (20); Invertebrate: Daphnia magna 24-hour LC₅₀: 800,000 ug/L (21).
- C. Effects on plants
 - C1. Phytotoxicity -- Data not available
 - C2. Uptake -- Data not available
 - C3. Metabolism -- Data not available
- VI. STANDARDS AND REGULATIONS
 - A. Health

TLV: TWA: 25 ppm or 100 mg/m³; STEL: 100 ppm or 400 mg/m³ (22).

CYCLOHEXANONE (cont.)

B. Environmental

Reported in EPA TSCA Inventory 1983.

Cyclohexanone has a statutory reportable quantity (RQ) of 1 lb under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (23).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (24).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (26).

C. Other Disposal Practices Employed

Burn in a chemical incinerator equipped with an afterburner and scrubber (27).

Spray into incinerator or burn in paper packaging. Additional flammable solvent may be added (6).

AEHA: NSN 6810-00-234-1992, 664-0055, 695-3801, 962-1873

Dispose of through a commercial contractor (27).

The Holston AAP Installation Assessment (28) indicates that open burning is the only Army approved method for disposal of explosive wastes. Solvents containing up to 80-90% water are burned in clay lined pits at Holston.

VIII. REFERENCES

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CYCLOHEXANONE (cont.)

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DI-n-PROPYL ADIPATE

Update of Atlantic Research Corporation Study

SUMMARY OF PREVIOUS STUDY

The Army's need for research on the toxicological and environmental hazards of di-n-propyl adipate is reported in A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. The report states that the compound has a low acute toxicity to mammals (g/kg), but that it has been shown to be teratogenic in rats receiving an acute dose. No information was found in the literature on the environmental fate of di-n-propyl adipate or on its toxicity to aquatic life, to microorganisms or to plants.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{12}H_{22}O_4$

Molecular Weight: 230.34 (1)

Structural Formula: $CH_3CH_2CH_2OCO(CH_2)_4COOCH_2CH_2CH_3$

B. Alternate Names and Registry Numbers

CAS Registry Number: 106-19-4

CA Name (9CI): Hexanedioic acid, dipropyl ester

CA Name (8CI): Adipic acid, dipropyl ester

RTECS Number: AV1740000

Other significant synonyms: Dipropyl hexanedioate

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Colorless (1)

Odor: Data not available

Boiling Point: $143-5^\circ$ at 10 mm Hg. (1)

DI-n-PROPYL ADIPATE (cont.)

Freezing Point: -20.3° (1)

Solubilities

Water: Insoluble (1)

Nonaqueous Solvents: Soluble in ethanol and ether (1)

Melting Point: Data not available

Octanol Water Partition Coefficient: $\log P = 2.88$ (estimated)

Hygroscopicity: Data not available

Specific Gravity: 0.979 (1)

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Plasticizer in rocket propellants (1)

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

A gas chromatographic method of analysis has been reported that is in the semi-micro range. The oven was temperature programmed and a flame ionization detector was used (2).

DI-n-PROPYL ADIPATE (cont.)

B. Limit of Detection

Data not available

IV. HEALTH EFFECTS

No information updating that in the ARC report was located.

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of di-n-propyl adipate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in the EPA TSCA Inventory 1980.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (3).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (4).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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DIAZODINITROPHENOL

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_2N_4O_5$

Molecular Weight: 210 (1)

Structural Formula: See Exhibit 18-1

B.1 Alternate Names and Registry Numbers (TSCA listing)

CAS Registry Number: 4682-03-5

Deleted CAS Registry Numbers: 90030-95-8; 7008-81-3; 28655-69-8

CA Name (9CI): 2,4-Cyclohexadien-1-one, 6-diazo-2,4-; (7CI) dinitro-

CA Name (8CI): Benzenediazonium, 2-hydroxy-3,5-dinitro-, hydroxide, inner salt

RTECS Number: Data not available

Other Significant Synonyms: DDNP

B.2 Alternate Names and Registry Numbers (RTECS listing)

CAS Registry Number: 87-31-0

CA Name (9CI): 1,2,3-Benzoxadiazole, 5,7-dinitro-

CA Name (8CI): Same

RTECS Number: DM2600000

Other Significant Synonyms: DDNP

C. Chemical and Physical Properties

Physical State: Crystalline solid, needles (1)

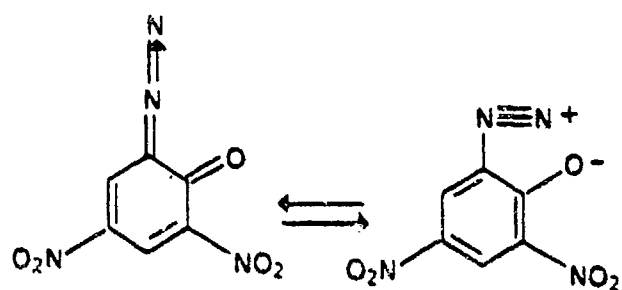
Color: Yellow (1)

Odor: Data not available

Melting Point: 157°C

DIAZODINITROPHENOL (cont.)

EXHIBIT 18-1



CAS No. 87-31-0

CAS No. 4682-03-5

DIAZODINITROPHENOL (cont.)

Solubilities:

Water: 0.08% at 25°C (2)

Nonaqueous Solvents: Soluble in nitroglycerin, nitrobenzene, aniline, pyridine, concentrated HCl and most organic solvents (1).

Solubility at 50°C in percentages (W:W) (1): Ethyl Acetate - 2.45%; Methanol - 1.25%; Ethanol - 2.43%; Ethylenedichloride - 0.79%; Carbon tetrachloride - trace; Chloroform - 0.11%; Benzene - 0.23%; Toluene - 0.15%; Petroleum ether - insoluble (at 20°C); Ethyl ether - 0.08% (at 30°C); Carbon disulfide - trace (at 30°C).

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: 0.04 at 90% relative humidity at 30°C (1)

Density (Crystal): 1.63 g/cc (1)

Volatility: Nonvolatile (1); unaffected; no weight loss at 50°C 30 months (2)

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: 3243 cal/g (1); 2243 cal/g (2)

Reactivity: Destroyed by 0.5% sodium hydroxide (2).

Stability: Stable after wet storage for five months (2). Explodes when shocked or heated to 180°C.

Flammability: Data not available

II. USES

A. Army Unique Use

Percussion caps (1)

B. Other Uses

Primary charge in blasting caps.

DIAZODINITROPHENOL (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Bratin et al. (3) described a reductive/oxidative electrochemical detection method with liquid chromatography that is sensitive and highly selective for explosive nitramine and nitrate compounds and diphenylamines.

B. Limit of Detection

Picomole range (3)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF DIAZODINITROPHENOL

Chemical	Species	Route	Effects	Reference
Diazodinitrophenol			Unknown	(4)
2,4-Dinitrophenol	Human	oral	LD ₅₀ : 36 mg/kg	(4)
	Human	dermal	Yellow staining of skin; may cause primary irritation or allergic sensitivity	(5)
	Human	systemic	Disruption of oxidative phosphorylation causing increased metabolism, oxygen consumption, and heat production; chronic exposure may result in kidney and liver damage and cataract formation	(5)
	Rat	oral	LD ₅₀ : 30 mg/kg	(4)
	Rat	intra-peritoneal	LD ₅₀ : 20 mg/kg	(4)
	Rat	subcutaneous	LD ₅₀ : 25 mg/kg	(4)
	Guinea pig	dermal	LD ₅₀ : 700 g/kg	(4)
	Wild birds	oral	LD ₅₀ : 13 mg/kg	(4)

DIAZODINITROPHENOL (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of diazodinitrophenol.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (6).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (7).

C. Other Disposal Practices Employed

Data not available

DIAZODINITROPHENOL (cont.)

VIII. REFERENCES

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DICHLORODIMETHYLEHYDANTOIN

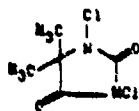
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_5H_6Cl_2N_2O_2$ (1)

Molecular Weight: 197.03 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 118-52-5

Deleted CAS Registry Number: 55945-60-3

CA Name (9CI): 2,4-Imidazolidinedione, 1,3-dichloro-5,5 dimethyl-

CA Name (8CI): Hydantoin, 1,3-dichloro-5,5-dimethyl-

RTECS Number: MU0700000

Other Significant Synonyms: Dantoin, dichlorantin, N'N'-dichloro-5,5-dimethylhydantoin

C. Chemical and Physical Properties

Physical State: Crystalline, four-sided, pointed prisms (1)

Color: Data not available

Odor: Data not available

Melting Point: $132^{\circ}C$; sublimes at $100^{\circ}C$; turns brown and conflagrates at $212^{\circ}C$ (1).

Solubilities:

Water: 0.21% at $25^{\circ}C$; 0.6% at $60^{\circ}C$ (1)

Nonaqueous Solvents: Freely soluble in chlorinated and highly polar solvents at $25^{\circ}C$: chloroform 14%, methylene chloride 30%, carbon tetrachloride 12.5%, ethylene dichloride 32%, sym-tetrachlorethane 17%, benzene 9.2% (1).

Octanol Water Partition Coefficient: $\log P = 1.63$ (estimated)

DICHLORODIMETHYLHYDANTOIN (cont.)

Hygroscopicity: Data not available

Density (Crystal): 1.5 g/cc (1)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: On contact with water, especially hot water, hypochlorous acid is liberated; at pH 9, nitrogen chloride is formed (1).

Stability: Dry crystals can be stored without much loss of available chlorine; after 14 weeks at 60°C, the chlorine loss was 1.5% (1).

Flammability: Data not available

II. USES

A. Army Unique Use

Military anti-mildew agent

B. Other Uses

Chlorinating agent, disinfectant, industrial deodorant; in water treatment; active ingredient of powder laundry bleaches; intermediate for amino acids, drugs, insecticides; stabilizer for vinyl chloride polymers and a polymerization catalyst (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

No chemical means of detection was found in a search of Chemical Abstracts dating back to 1967.

B. Limit of Detection

Data not available

DICHLORODIMETHYLHYDANTOIN (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF 1,3-DICHLORO-5,5-DIMETHYLHYDANTOIN

Chemical	Species	Route	Effects	Reference
1,3-Dichloro-5,5-dimethylhydantoin	Animals	local	Caustic and corrosive to the eyes, skin, and mucous membranes; may produce severe burns and irreversible cellular damage in the eye	(2)
	Animals	inhalation	Irritating to lungs	(2)
		oral	LD ₅₀ : 542 mg/kg	(3)
	Rabbit	oral	LD ₅₀ : 1,520 mg/kg; behavioral and pulmonary system effects	(3)
	Guinea pig	oral	LD ₅₀ : 1,350 mg/kg; behavioral and pulmonary system effects	(3)
Hypochlorous acid (available chlorine)	Human	local	Highly irritating to skin, eyes, and mucous membranes	(4)
	Human	ingestion	Irritation and corrosion of mucous membranes with pain and vomiting; a fall in blood pressure, delirium, and coma may occur	(5)
	Human	inhalation	Coughing, choking; may cause severe respiratory tract irritation and pulmonary edema	(5)

DICHLORODIMETHYLHYDANTOIN (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF

1,3-DICHLORO-5,5-DIMETHYL-HYDANTOIN

Test System	Dose	Effects	Reference
Rat embryo cells	6,300 ng/plate	Oncogenic transformation	(3)

V. ENVIRONMENTAL EFFECTS

Log BCF = 1.01 Estimated

No other information was found regarding the environmental fate or effects of dichlorodimethylhydantoin.

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 0.2 mg/m³; STEL 0.4 mg/m³ (3)

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended on an interim basis by the U.S. Navy in their Consolidated Hazardous Item List for a "Mildew Resistant Compound," a related compound used for a related purpose, are to bury in a hazardous waste disposal site (6).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

The material is ignited in the presence of sodium carbonate and slaked lime (calcium hydroxide). The substance is mixed with vermiculite and then with dry caustics, wrapped in paper and burned in a chemical incinerator equipped with an afterburner and scrubber (7).

DICHLORODIMETHYLHYDANTOIN (cont.)

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DICHLOROPHENE

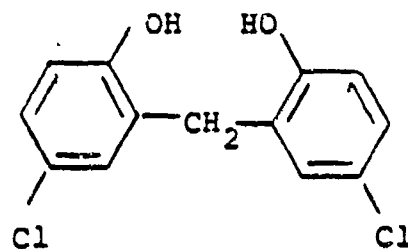
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{13}H_{10}Cl_2O_2$

Molecular Weight: 269.13

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 97-23-4

CA Name (9CI): Phenol], 2,2'-methylenebis [4-chloro-

CA Name (8CI): Same

RTECS Number: SM0175000

Other significant synonyms: [(Dihydroxydichloro)diphenyl]methane; 2,2'-dihydroxy-5,5'-dichlorodiphenylmethane; 5,5'-dichloro-2,2'-dihydroxydiphenylmethane; bis[5-chloro-2-hydroxyphenyl]methane; di[5-chloro-2-hydroxyphenyl]methane

C. Chemical and Physical Properties

Physical State: Crystalline

Color: Data not available

Odor: Data not available

Melting Point: 177-178°C (1)

DICHLOROPHENE (cont.)

Solubilities:

Water: Insoluble. Soluble in alkaline aqueous solutions with decomposition (2).

Nonaqueous Solvents: Soluble in methanol, isopropyl alcohol and petroleum ether (2).

Octanol Water Partition Coefficient: $\log P = 4.72$ (estimated)

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Military anti-mildew agent

B. Other Uses

Fungicide and bactericide; texture preservative; some dermatological and cosmetic applications; veterinary medicine; plant root growth inhibitor.

DICHLOROPHENE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

High pressure liquid chromatography has been reported by Shah et al. (4) as a good method for quality control in veterinary products. A reverse-phase column was used with a variable wave-length detector set at 290 nm. The mobile phase was methanol-water (75:25). This is not a method for trace analysis, but could be adapted for environmental samples. Thin-layer chromatography has also been reported for quality control in the pharmaceutical industry.

B. Limit of Detection

Data not available

DICHLOROPHENE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF DICHLOROPHENE

Species	Route	Dose/Duration	Effects	Reference
Human	NS*	NS	Cramps, diarrhea	(5)
Human	dermal	0.25% in a dermatologic preparation (Unna's Boot material)	Caused allergic dermatitis; confirmed by patch tests of dichlorophene in petrolatum	(6)
Human	dermal	1% in yellow petrolatum (patch)	22/4320 eczema patients had weak positive sensitization reactions; no patients showed irritation reactions	(3)
Human	dermal	Induction: 20% in petrolatum; challenge: 5% in petrolatum (patch)	1/110 individuals showed signs of sensitization; 0/208 at 5% induction concentration	(7)
Rat	oral	2,000 ppm in diet for 90 d	No toxicity	(8)
Rat	oral	2,690 mg/kg	LD ₅₀	(9)
Rat	intravenous	17 mg/kg	LD ₅₀	(9)
Mouse	oral	1,000 mg/kg	LD ₅₀	(9)
Guinea pig	oral	1,250 mg/kg	LD ₅₀	(9)
Guinea pig	intradermal, topical	Induction: 5% in propylene glycol intradermally + 25% in yellow petrolatum topically; challenge: 1% in yellow petrolatum topically (patch)	Weak sensitizer	(3)

* Not specified

DICHLOROPHENE (cont.)

TABLE IV-1. TOXICITY OF DICHLOROPHENE (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Guinea pig	dermal	25% in yellow petrolatum	Not irritating	(3)
Rabbit	dermal	500 mg/24 hr	Mild irritation	(9)
Rabbit	eye	50 ug/24 hr	Severe irritation	(9)
Dog	oral	2,000 mg/kg	LD ₅₀	(9)
Mammal	NS*	1,000 mg/kg	LD ₅₀	(9)

* Not specified

TABLE IV-2. MUTAGENICITY OF DICHLOROPHENE

Test system	Dose	Effects	Reference
<u>Salmonella typhimurium</u> (TA1535)	50 nmol/plate	Mutagenic without Aroclor-induced rat liver S9	(10)
<u>Drosophila Melanogaster</u> Basic test	12.5 mM; oral (approx. LD ₅₀)	No increase in frequency of sex-linked recessive lethal mutations	(10)
Micronucleus test on mouse bone marrow	27, 54, or 81 mg/kg x2; ip	No increase in frequency of micronuclei	(10)

DICHLOROPHENE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Log BCF: 3.36 (estimated)

A2. Transformation -- Data not available

A2a. Biodegradation -- After 3 weeks adaptation at 10 to 20 mg/L at 22°C: under aerobic conditions, 25% degradation when dichlorophene is sole carbon source, 50% degradation with synthetic sewage; under anaerobic conditions, no degradation, even with synthetic sewage (8).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Dichlorophene added to the food of ducks daily for 5 days at 0.5 g/kg body weight did not adversely affect the general health or the serum protein levels (total and individual protein fractions), even though the dose was the maximum therapeutic dose used for treating helminthic infections in ducks (11).

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- The algicidal doses of dichlorophene to four species of blue-green algae which are common in swimming pools, impoundments, wastewater effluents, and receiving waters at pH 6.5 ranged from 4.0 to 9.0 ppm. The algicidal dosage increased with increasing pH (12).

DICHLOROPHENE (cont.)

- B7. Aquatic species, fish and invertebrates -- Harlequin fish (Rasbora heteromorpha) flow-through bioassay: 24-hour LC_{50} : 5.4 mg/L (sodium salt); 48-hour LC_{50} : 4.8 mg/L (sodium salt); 96-hour LC_{50} : 3.6 mg/L (sodium salt) (8).

C. Effects on plants

- C1. Phytotoxicity -- Dichlorophene is used for inhibiting root growth and preventing root twisting in containerized seedlings of pine and spruce (3).

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Based on the disposal practices recommended by the U.S. Navy for a similar compound, "mildew preventive," dichlorophene should be buried in a hazardous waste disposal site (13).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber (14).

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DIETHYLENE GLYCOL DINITRATE (DEGN)

Much of the available data on diethylene glycol dinitrate has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_4H_8N_2O_7$

Molecular Weight: 196.14

Structural Formula: $O_2NOCH_2CH_2OCH_2CH_2ONO_2$

B. Alternate Names and Registry Numbers

CAS Registry Number: 693-21-0

CA Name (9CI): Ethanol, 2,2'-oxybis-dinitrate

CA Name (8CI): Diethylene glycol, dinitrate

RTECS Number: ID6825000

Other Significant Synonyms: DEGN, diglycol nitrate, dinitroglycol

C. Chemical and Physical Properties

Physical State: Liquid

Color: Yellow

Odor: Data not available

Melting Point: $-11.3^{\circ}C$ (1)

Boiling Point: $161^{\circ}C$, Decomposes (2)

Solubilities:

Water: Slightly 0.40 g/100g ($20^{\circ}C$) and 0.60 g/100g ($60^{\circ}C$) (3).

Nonaqueous Solvents: Slightly soluble in alcohol and water soluble in ether (3). Insoluble in ether alcohol, 2:1 ether:alcohol, acetone (2).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

DIETHYLENE GLYCOL DINITRATE (DEGN) (cont.)

Density (Crystal): 1.377 (4)

Volatility: Data not available

Vapor Pressure: 0.0036 mm Hg 20°C

Specific Heat: Data not available

Reactivity: Reacts vigorously with oxidizing or reducing material (5).

Heat of Combustion: 2792 cal/g (4)

Stability: Relatively stable at room temperature (6)

Flammability: Highly explosive when shocked or exposed to heat.
Emits toxic fumes of NO when heated (5).

II. USES

A. Army Unique Use

Plasticizer in solid rocket propellants

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

In addition to the methods previously reported in the Atlantic Research Corporation Report, an HPLC/mass spectroscopy method for forensic and trace analysis is the most recent method for this compound. Yinon (1) described a custom-built mass spectrometer interfaced with a high pressure liquid chromatograph that can successfully analyze DEGN and other explosives.

B. Limit of Detection

Data not available

DIETHYLENE GLYCOL DINITRATE (DEGN) (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF DIETHYLENE GLYCOL DINITRATE* (7)

Species	Route	Dose/Duration	Effects
Human (workers in DEGDN and nitrogly- cerin-pro- ducing plant	inhalation	Above 5 mg/m ³	Coronary occlusion in 4 workers who died suddenly (29-47 yr old, 5-7 yr exposure); 37 of 45 other workers reported precordial pain, headaches, and rarely collapse conditions with loss of consciousness; signs of coronary sclerosis in 3, symptoms of intermediary coronary syndrome in 8, and 1 myocardial infarction; cholesterol blood level was at the upper borderline of normal (220 mg%) in most and reached 300 mg% in some
Rat	oral	777 mg/kg	LD ⁵⁰
White rats	oral in veget- able oil	1,180 mg/kg	LD ⁵⁰ ; central nervous system damage and acute cyanosis
White rats (male)	oral	6x/wk for 6 mo: 0.05 mg/kg	No effects
		0.5 mg/kg	Minimum effective dose; changes in conditional reflex activity and immunobiological response
		5.0 mg/kg	Decrease in blood pressure by 5th to 6th month; change in the mitotic activity of the bone marrow
White mice	oral in veget- able oil	1,250 mg/kg	LD ⁵⁰ ; central nervous system damage and acute cyanosis
Guinea pig	oral in veget- able oil	1,250 mg/kg	LD ⁵⁰ ; central nervous system damage and acute cyanosis

* Information not included in the ARC report

DIETHYLENE GLYCOL DINITRATE (DEGN) (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF DIETHYLENE GLYCOL DINITRATE

Test System	Dose	Effects	Reference
<u>Escherichia coli</u> W3110/po1A ₋ , p3478/po1A DNA repair assay	100 ug- 10 mg	Not active with or without Aroclor 1254- induced rat liver S9	(8)
<u>Salmonella</u> <u>typhimurium</u> TA100, TA1535, TA1537, TA1538	NS*	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(8)
<u>Saccaromyces</u> <u>cerevisiae</u>	NS	Did not produce mitotic recombination with or without Aroclor 1254- induced rat liver S9	(8)

* Not specified

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of diethylene glycol dinitrate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in the EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and

landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (9).

B. Alternate Disposal Practices Under Consideration by the Army

Future plans of disposal of waste explosives and propellants are projected to emphasize fluid bed incineration. This method has been tested successfully by ARRADCOM and is planned to be used at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Amunition Depot (10).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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DIETHYLENE GLYCOL DINITRATE (DEGN) (cont.)

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DIETHYLENE TRIAMINE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_4H_{13}N_3$

Molecular Weight: 103.17

Structural Formula: $H_2NCH_2CH_2NHCH_2CH_2NH_2$

B. Alternate Names and Registry Numbers

CAS Registry Number: 111-40-0 (current)

Deleted CAS Registry Numbers: 59135-90-9, 54018-92-7, 26915-78-6
53303-76-7, 8076-55-9

CA Name (9CI): 1,2-Ethanediamine, N-(2-aminoethyl)-

CA Name (8CI): Diethylenetriamine

RTECS Number: IE1225000

Other Significant Synonyms: 3-azapentane-1,5-diamine, bis[.beta.-aminoethyl]amine, 2,2'-diaminodiethylamine, bis(2-aminoethyl)amine, N,N-bis(2-aminoethyl)amine, 1,4,7-triazaheptane, 1,5-diamino-3-azapentane

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Yellow (1)

Odor: Ammoniacal (2)

Melting Point: $-39^{\circ}C$ (1)

Boiling Point: $208^{\circ}C$ (1)

Solubilities:

Water: Miscible (1)

Nonaqueous Solvents: Miscible with alcohol; insoluble in ether; soluble in ligroin (1).

Octanol Water Partition Coefficient: $\log P = -1.27$ (estimated)

DIETHYLENE TRIAMINE (cont.)

Hygroscopicity: Hygroscopic (1)

Specific Gravity: 0.9542 (1)

Volatility: Data not available

Vapor Pressure: 0.2 Torr at 20°C; 0.75 Torr at 20°C (3)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Corrosive

Stability: Stable (4)

Flammability: Slight; combustion requires preheating (4); flash point-101°C (2).

II. USES

A. Army Unique Use

A component of DS2, a decontaminant for chemical agents (5).

B. Other Uses

Reactive hardener in epoxy formulations (6). Solvent for sulfur, acid gases, resins, dyes, fuel component.

III. ANALYTICAL METHODS

A. Best Acceptable Method

Ng (6) recently reported a gas chromatographic/mass spectroscopic method for the detection of the tert-butyldimethylsilyl derivative.

B. Limit of Detection

Data not available

DIETHYLENE TRIAMINE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF DIETHYLENETRIAMINE (DETA)

Species	Route	Dose/Duration	Effects	Reference
Human	inhalation	NS*	Moderate, temporary irritation	(7)
		long exposure	May cause asthma	(7)
Human	skin	short exposure	Smarting and first-degree burns	(7)
		long exposure	May cause secondary burns	(7)
Human	skin	NS*	Can produce rash and sensitization	(7,8)
Human (2 workers)	skin	10 and almost 20 yr	Allergic contact dermatitis from DETA in a detergent	(9)
Human	eye	NS*	Produces burns	(7)
Human	NS	NS*	"There are existing data which indicate a theoretical potential for the conversion of DETA to nitrosamines in the environment and that persons may be exposed to these nitrosamines as a result of release of DETA to the environment. Nitrosamines have been shown to be carcinogenic."	(10)
Rat	oral	1,080 mg/kg	LD ₅₀ : convulsions	(11)
Rat	intra-peritoneal	74 mg/kg	LD ₅₀ : convulsions, peritonitis	(11)
Rat	inhalation	Concentrated vapor and 300 ppm	No effect	(8)

* Not specified

DIETHYLENE TRIAMINE (cont.)

TABLE IV-1. TOXICITY OF DIETHYLENETRIAMINE (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Mouse	intra-peritoneal	71 mg/kg	LD ₅₀ ; convulsions, peritonitis	(11)
Guinea pig	skin	162 mg/kg	LD ₅₀	(11)
Rabbit	skin	10 mg/24 hr	Severe irritation	(11)
Rabbit	skin	500 mg (open)	Moderate irritation	(11)
Rabbit	skin	1,090 mg/kg	LD ₅₀	(11)
Rabbit	eye	750 ug	Severe irritation	(11)

* Not specified

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF DIETHYLENETRIAMINE

Test System	Effects	Reference
<u>Salmonella typhimurium</u>	Nonmutagenic with or without Aroclor 1254-induced rat or Syrian hamster liver S9	(12)
<u>Salmonella typhimurium</u> TA100	Slight mutagenic activity	(13)
<u>Salmonella typhimurium</u> TA100, TA1535	Mutagenic without metabolic activation; may be due to impurity	(14)

DIETHYLENE TRIAMINE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2a. Biodegradation -- Bio-oxidation in fresh water in 15 days: 4% with non-acclimated microbial cultures, up to 70% at 20 days with acclimated microbial cultures (15).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- ThOD: 1.55 (15)

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

B7. Aquatic species, fish and invertebrates -- Brine shrimp $TL_m = 710$ mg/L at 24 hours (15)

C. Effects on plants

C1. Phytotoxicity -- Data not available

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

DIETHYLENE TRIAMINE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA(skin): 4 mg/m³ or 1 ppm (16).

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for "Decontaminating Agent," a related mixture used for a related decontamination, are to bury in a sanitary landfill (17).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Emits highly toxic vapors when burned. Solution can be sprayed into an incinerator with afterburner and scrubber (16).

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DINITROPHENYL AZIDE

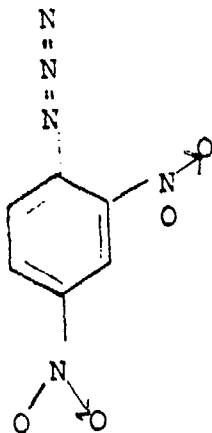
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_3N_5O_4$

Molecular Weight: Data not available

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 4096-88-2

CA Name (9CI): Benzene, 1-azido-2,4-dinitro-

CA Name (8CI): Same

RTECS Number: CY6610000

*Under Benzene, 1-azido-2,4-dinitro- on the ICIS System the following information was obtained:

CAS Registry Number: 17508-17-7

CA Name (9CI): Hydroxylamine, O-(2,4-dinitrophenyl)-

DINITROPHENYL AZIDE (cont.)

CA Name (8CI): Same as above.

RTECS Number: CY6610000

Other Significant Synonyms: Benzene, 1-azido-2,4-dinitro,
Dinitrophenylazide, DNPA

The structure displayed in the CIS System is not an azide; the structure displayed in CAS under that Registry Number is not the same, but it is also not an azide. For sake of completeness, this Registry Number should be included in further search schemes with the caveat that the search results will have to be screened for the correct compound.

C. Chemical and Physical Properties

Physical State: Data not available

Color: Data not available

Odor: Data not available

Melting Point: Data not available

Solubilities:

Water: Data not available

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: $\log P = 3.22$ (1), 3.50 (2), 3.59 (3), 3.72 (2)

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

DINITROPHENYL AZIDE (cont.)

II. USES

A. Army Unique Use

Initiator for explosives.

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

No methods of analysis were found in Chemical Abstracts, searching back to 1967.

B. Limit of Detection

Data not available

DINITROPHENYL AZIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF DINITROPHENYL AZIDE

Chemical	Species	Route	Effects	Reference
Dinitrophenyl azide			No toxicity data located other than mutagenicity (see following table)	
2,4-Dinitro-aniline	NS*	NS	Irritating to skin and mucous membranes; highly toxic if absorbed	(4)
	Rat	oral	LD ₅₀ : 418 mg/kg	(5)
	Rat	intra-peritoneal	LD _{Lo} : 250 mg/kg	(5)
	Rabbit	eye	Severe irritation	(5)
Dinitrobenzene (all isomers)	NS	NS	Anoxia due to methemoglobin formation; respiratory tract irritation and anemia in prolonged exposure	(6)

* Not specified

DINITROPHENYL AZIDE (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF DINITROPHENYL AZIDE*

Test system	Dose	Effects	Reference
<u>Salmonella</u> <u>typhimurium</u> (TA98, TA100, TA1535, TA1537, TA1538)	5-20 ug/plate	Mutagenic without liver microsomes	(7)
<u>Escherichia</u> <u>coli</u> (WP2s)	1-400 ug/plate	Nonmutagenic	(7)

* 2,4-Dinitrophenyl azide

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of dinitrophenyl azide.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (8).

DIPHENYLAMINE

Much of the available data on diphenylamine has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

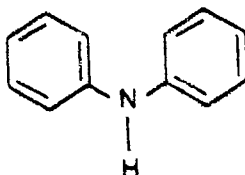
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $(C_6H_5)_2NH$

Molecular Weight: 169.24

Structural formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 122-39-4

CA Name (9CI): Benzenamine, N-phenyl

CA Name (8CI): Diphenylamine

RTECS Number: JJ 7800000

Other Significant Synonyms: Aniline, N-phenyl; N,N-diphenylamine; N-phenylaniline; N-phenylbenzenamine.

C. Chemical and Physical Properties

Physical State: crystals

Color: colorless

Odor: floral (1)

Melting Point: 52.85°C

DIPHENYLAMINE (cont.)

Boiling Point: 302°C at 760 mmHg (2)

Solubilities:

Water: Slightly soluble-0.03 g/100 g at 2°C (3)

Nonaqueous Solvents: Soluble in alcohol 44 g/100 g, very soluble in ether. Methyl alcohol 57.5 g/100 g (3). Acetone-very soluble.

Very soluble in carbon disulfide (4), glacial acetic acid.

Octanol Water Partition Coefficient: Log P = 3.5

Hygroscopicity: Data not available

Density (Crystal): 1.1559 g/cc (5)

Volatility: Data not available

Vapor Pressure: 1mm Hg at 108.3°C (4)

Flash Point: 153°C (5)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: inflammable

Stability: Data not available

Flammability: Data not available

Vapor Density: 5.82 g/m³

Autoignition temp: 619.67°C (4).

II. USES

A. Army Unique Use

Used as an explosive and a stabilizing compound for propellants and explosives.

B. Other Uses

Manual dyes; stabilizing nitrocellulose explosives and celluloid. In analytical chemistry for the detection of NO₃⁻, ClO₂⁻ and other oxidizing substances with which, in the presence of H₂SO₄, it gives a deep-blue color. In veterinary medicine, it is used topically in anti-screwworm mixtures and in tests for nitrate and nitrite poisoning.

DIPHENYLAMINE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

High pressure liquid chromatography has become the method of choice for this stabilizer for quality control of propellants. Bender (6) reported a qualitative and quantitative determination using UV (ultraviolet) or TEA (thermal energy analyzer) detectors. Barth and Zierath (7) reported HPLC, TLC, (thin-layer chromatography) and HP-TLC methods for analysis in double-based powers. For determining diphenylamine in waste water, Svechnikova (8) reported a chloroform extraction followed by gas chromatography for the analysis of effluents from antioxidant manufacturing. The applicability of this method to propellant manufacturing effluent cannot be extrapolated.

B. Limit of Detection

Data not available

DIPHENYLAMINE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF DIPHENYLAMINE^a

Species	Route	Dose/Duration	Effects	Reference
Human	oral, dermal, inh	NS*	Headache; fatigue; cyanosis; fast pulse; hypertension; bladder injury; chemical asphyxia from methemoglobin- emia	(9)
Human	inh or contact with dust	NS	Eye and mucous membrane irritation	(9)
Human	dermal	1% in petrolatum (patch)	No sensitization or irritation reactions	(10)
Rat	oral	1.2-3.2 g/kg	LD ₅₀	(10)
Rat	oral	1.6 g/kg	Decreased hemoglobin and oxyhemoglobin levels; increased methemoglobin and Heinz-body formation	(10)
Rat	oral	2.5% in feed for 3-6 wk to 0.1% in feed for 2 yr	Renal cystic disease	(10)
Rat	oral	7,500 mg/kg given during gestation days 17-22	TD _{Lo} for developmental abnormalities	(10)
Rat	oral	3,000 mg/kg	LD _{Lo}	(11)
Guinea pig	oral	300 mg/kg	LD ₅₀	(11)
Rabbit	dermal (intact or for 24 hr abraded skin)	full strength (patch)	Not irritating	(10)

DIPHENYLAMINE (cont.)

TABLE IV-1 TOXICITY OF DIPHENYLAMINE (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Dog	oral	1% in feed for 2 yr (99.9% pure)	Severe growth inhibition, low hemoglobin levels and red cell counts, crenated red cells, increase in red cell fragility, fatty livers, hemosiderosis of the spleen, kidney, and bone marrow	(10)
Cat	oral	1 mmol/kg in aqueous suspension	Methemoglobin formation	(10)

a. Not included in ARC Report

* Not specified

DIPHENYLAMINE (cont.)

TABLE IV-2 MUTAGENICITY AND RELATED EFFECTS OF DIPHENYLAMINE

Test System	Dose	Effects	Reference
<u>Escherichia coli</u> W3110/polA ⁻ , p3478/polA ⁻ , DNA repair assay	10 mg	100 ug-Not active with or without Aroclor 1254- induced rat liver S9	(12)
<u>Salmonella</u> <u>typhimurium</u> TA100, TA1535 TA1537, TA1538	NS*	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(12)
<u>S. typhimurium</u> (11 strains), <u>E. coli</u> (2 strains)	10,000- fold conc. range	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(12)
<u>Saccharomyces</u> <u>cerevisiae</u> D5	NS	Did not produce mitotic recombination with or without Aroclor 1254- induced rat liver S9	(12)
Primary rat hepatocyte cultures	up to 1 mmol/mL	Did not induce un- scheduled DNA synthesis	(13)
Rat kidney cells infected with murine sarcoma virus	2.5-20 ug/mL	Did not significantly increase the frequency of viral transformation with or without Aroclor- induced rat liver S9	(14)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport — Data not available

A1a. Adsorption — Data not available

A1b. Volatilization — Data not available

DIPHENYLAMINE (cont.)

- Alc. Leachability -- Diphenylamine's relatively low solubility in water (18 mg/L at 10°C) and moderately high octanol/water partition coefficient indicate a relatively high tendency to associate with sediments in the hydrosphere and to migrate slowly in soils containing organic matter (15).
- Ald. Bioaccumulation -- Bioconcentration factor (BCF) = 30, determined with the fathead minnow (Pimephales promelas) in 32-day exposure (16).
- A2. Transformation -- Data not available
- A2a. Biodegradation -- Diphenylamine undergoes progressive oxidative metabolism by sewage sludge organisms. Some of the metabolites (4-hydroxy-diphenylamine, indole and aniline) are more acutely toxic than the parent compound, but these metabolites are not persistent in the sludge mixed liquor after they are formed. After 6 hours incubation (common digestion period in sewage treatment plants) the microbial degradation of diphenylamine was incomplete, with more than 35% undegraded (17).
- A2b. Hydrolysis -- Data not available
- A2c. Photolysis -- Photochemical reactions may be possible since diphenylamine does absorb light around 285 nm (15).
- A2d. Other chemical reaction -- COD: 90% of ThOD (0.05 Cr₂O₇)
ThOD: 2.39 (18). When used as a propellant stabilizer, diphenylamine undergoes oxidation with nitrous acid to form diphenyl-N-nitrosamine. Subsequent reactions with nitrogen oxides in the propellants can take place (if mineral acids are present) with the eventual formation of 2,4,4'-trinitrodiphenylamine (15).
- A2e. Half-life -- Data not available
- B. Effects on Animals
- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available

DIPHENYLAMINE (cont.)

- B6. Microorganisms, aquatic and soil -- Impact on biodegradation processes:
At 100 mg/L, no inhibition of NH_3 oxidation by Nitrosomonas sp. (18).
In 7-day test at 25°C, 5 mg/L resulted in death of algae (unspecified) cultures (15). The median growth-inhibiting dose (ID_{50}) of diphenylamine to the ciliate Tetrahymena pyriformis was 25 $\mu\text{g/mL}$ (10). Diphenylamine was found to be inactive in bacterial DNA repair and reversion tests and yeast mitotic recombination assays made to assess the qualitative nature of the compound's genotoxic potential (12). Numerous studies have been conducted on the effect of diphenylamine on various biochemical reactions in microorganisms. Particular attention has been paid to the stimulation or inhibition of carotenoid (pigment) synthesis and the resulting altered photosensitivity of the organisms. Inhibition of growth has been noted for some organisms with concentrations of about 10^{-4} M. Several investigators have observed that diphenylamine is taken up in the plasma membrane and that certain adverse effects on the membrane result (15). Diphenylamine is applied to the surface of apples and pears to be kept in long cold storage to control the microorganisms associated with scald and rot (15).

- B7. Aquatic species, fish and invertebrates -- Bluegill sunfish: 96-hour LC_{50} = 1.18 mg/L at 21°C. (Cyclocypris sp.): 48-hour LC_{50} = 2.53 mg/L at 21°C (15).

C. Effects on Plants

- C1. Phytotoxicity -- Diphenylamine has been shown to affect the foliar morphogenesis, germination, rhizogenesis, heteroblastic development and senescence in the tomato (Lycopersicon esculentum Mill) (15).
- C2. Uptake -- Data not available
- C3. Metabolism -- Diphenylamine has been shown to be an effective inhibitor of overall carotene synthesis in a soluble tomato plastid enzyme system; and in pumpkin cotyledons, the compound also reduced carotene accumulation (15).

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 10 mg/m^3
STEL 20 mg/m^3 (11)

The Food and Drug Administration (21 CFR 175 and 176) has placed restrictions on the use of diphenylamine in food packaging materials (15).

DIPHENYLAMINE (cont.)

B. Environmental

Reported in EPA TSCA Inventory, 1980.

The EPA has established (40CFR 180.190) tolerances for the residues of the fungicide diphenylamine as follows:

10 ppm in or on apples from preharvest or postharvest use, including use of impregnated wraps, for scald control;

Zero (0) in milk and meat (apple processing residues - cores, skins, etc. - are sometimes used as a feed supplement for cows) (15).

DIPHENYLAMINE (cont.)

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (18).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (19).

C. Other Disposal Methods Employed

Disposal Method Suggested: Burn in admixture with flammable solvent in furnace equipped with afterburner and scrubber (20).

SAFETY AND CONTROL MEASURES. Disposal personnel handling these items shall wear safety glasses, impervious gloves, and a protective laboratory coat. A NIOSH respirator approved for this item should be available.

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ETHYL CENTRALITE

Much of the available data on ethyl centralite has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

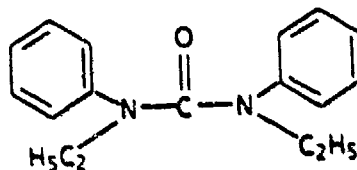
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{17}H_{21}ON_2O$

Molecular Weight: 266.39

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 85-98-3

CA Name (9CI): Urea, N,N'-diethyl-N,N'-diphenyl

CA Name (6CI): Carbanilide, N,N'-diethyl

RTECS Number: FE0350000

Other Significant Synonyms: Bis(N-ethyl-N-phenyl)urea; carbamate; centralite; centralite-1; sym-diethyldiphenylurea; centralite; urea, 1,3-diethyl-1,3-diphenyl.

C. Chemical and Physical Properties

Physical State: Crystalline solid (1)

Color: White (1)

Odor: Peppery (1)

Melting Point: 79°C (1)

ETHYL CENTRALITE (cont.)

Boiling Point: 325-330°C (1)

Solubilities:

Water: Insoluble

Nonaqueous Solvents: Soluble in organic solvents.

Octanol Water Partition Coefficient: Log P = 5.02 (2)

Hygroscopicity: Data not available

Density (Crystal): 1.12 g/cc at 20°C (3)

Volatility: Data not available

Vapor Pressure: Data not available

Flash Point: 150°C

Specific Heat: Data not available

Heat of Combustion: 8409.3 cal/g (4)

Reactivity: Data not available

Stability: Severe explosion hazard when shocked or heated (1)

Flammability: Data not available

II. USES

A. Army Unique Use

Stabilizer for nitrocellulose-based smokeless powder in rocket propellants (3).

B. Other Uses

Proposed retarder for preventing aging of vulcanized rubber (5).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Little work has been done on the quantitative analysis of ethyl centralite at trace levels. Most methods have been developed for quality control and stability analysis of propellants. In addition to the methods described in the Atlantic Research Corporation report, there is a gas-liquid chromatography method by Alley and Dykes (6) reported in 1972 that successfully separated and identified the components of double-based propellants including ethyl centralite.

ETHYL CENTRALITE (cont.)

Alley and Dykes used a flame ionization detector and a silicone-based stationary phase.

Additionally, a high-pressure liquid chromatographic method was developed to study the stability of double-base powders. Ethyl centralite, along with 29 other components and derivatives, was detected under isocratic conditions within 35 minutes, or 50 minutes running a gradient (7). This method could possibly be adapted for trace analysis of environmental and other samples.

B. Limit of Detection

Data not available

IV. HEALTH EFFECTS

TABLE IV-1. MUTAGENICITY AND RELATED EFFECTS OF ETHYL CENTRALITE*

Test System	Dose	Effects	Reference
<u>E. coli</u> W3110/polA ⁺ , p3478/polA ⁻	100 ug- 10 mg	Not active with or without Aroclor 1254- induced rat liver S9	(8)
<u>S. typhimurium</u> TA100, TA1535, TA1537, TA1538	NS**	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(8)
<u>S. cerevisiae</u> D5	NS	Did not produce mitotic recombination with or without Aroclor 1254- induced rat liver S9	(8)

* Information not included in the ARC report

** Not specified

V. ENVIRONMENTAL EFFECTS

No information was found on the environmental fate or effects of ethyl centralite which would update the Atlantic Research Corporation document.

ETHYL CENTRALITE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Toxic (1)

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (9).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (10).

C. Other Disposal Practices Employed

Data not available

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ETHYLENE GLYCOL

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_2H_6O_2$ (1)

Molecular Weight: 62.07 (1)

Structural Formula: $HOCH_2CH_2OH$

B. Alternate Names and Registry Numbers

CAS Registry Number: 107-21-1

Deleted CAS Registry Number: 71767-64-1, 37221-95-7

CA Name (9CI): 1,2-Ethanediol

CA Name (8CI): Ethylene glycol

RTECS Number: KW2975000

Other Significant Synonyms: Glycol, monoethylene glycol, 1,2-dihydroxyethane, 2-hydroxyethanol

C. Chemical and Physical Properties

Physical State: Liquid (slightly viscous) (1)

Color: Clear

Odor: Sweet (2)

Melting Point: $-13^{\circ}C$ (1)

Boiling Point: $198^{\circ}C$ (1)

Solubilities:

Water: Miscible with water (1)

Nonaqueous Solvents: Miscible with lower aliphatic, alcohols, glycerol, acetic acid, acetone and similar ketones, aldehydes, pyridine and similar coal tar bases; slightly soluble in ether (1:200); practically insoluble in benzene and its homologs, chlorinated hydrocarbons, petroleum ether and oils (1).

Octanol Water Partition Coefficient: -1.93 to -1.36 (3,4)

ETHYLENE GLYCOL (cont.)

Hygroscopicity: Very hygroscopic, adsorbs twice its weight of water at 100% relative humidity (1).

Specific Gravity: 1.1088 (5)

Volatility: Data not available

Vapor Pressure: 0.05 Torr at 20°C (6), 0.12 Torr at 20°C (7),
0.2 Torr at 30°C (6)

Specific Heat: 0.561 cal/g/°C (1)

Heat of Combustion: Data not available

Reactivity: Reacts violently with chlorosulfonic acid and oleum (2)

Stability: May be explosive when heated (2)

Flammability: Slight, combustion requires preheating (8), flash point,
open cup: 111°C (8)

II. USES

A. Army Unique Use

Intermediate in the production of explosive ethylene glycol dinitrate.

B. Other Uses

Antifreeze; hydraulic brake fluids; industrial humectant; ingredient in electrolytic condensers, where it serves as solvent for boric acid and borates; solvent in the paint and plastics industry; formulation of printers' inks, stamp pad inks, inks for ball point pens; softening agent for cellophanes; stabilizer for soybean foam used to extinguish oil and gasoline fires; synthesis of safety explosives, glyoxal, unsaturated ester-type alkyd resins, plasticizers, elastomers and synthetic fibers (Terylene and Dacron) and synthetic waxes (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Gas chromatography would be the method of choice and many have been reported. Two of the most recent methods apply to environmental and health effects studies respectively. Nevinnaya and Kofanov (9) formed the acetyl derivative, and used an XE-60 column with flame ionization detection to determine ethylene glycol in wastewater. A capillary

ETHYLENE GLYCOL (cont.)

gas chromatographic method has been developed by Smith (10) to determine ethylene glycol in human blood serum. Smith formed the butylboronate derivative before injection onto a methylsilicone bonded fused silica column.

B. Limit of Detection

Nevinnaya and Kofanov reported 10 ppb as the lower limit of detection (9).

ETHYLENE GLYCOL (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ETHYLENE GLYCOL

Species	Route	Dose/Duration	Effects	Reference
Human	ingestion	1.4 mL/kg (100 mL)	Approx. lethal dose	(1)
Human	ingestion	NS*	Transient stimulation of the central nervous system followed by depression; vomiting, drowsiness, coma, respiratory failure, convulsions; exudative pathological changes in the brain; renal damage which may proceed to anuria, uremia, death	(1, 11)
Human	ingestion	"Sip" to approx. 120 mL (antifreeze solution)	Neuromuscular disturbance with myositis after deposition of calcium oxalate crystals; circulatory depression with rapid breathing, cyanosis, and edema of the lungs; renal failure; death after consumption of 90-120 ml	(12)
Human	ingestion	710 mg/kg	LD _{Lo}	(13)
Human (child)	ingestion	7,400 mg/kg	TD _{Lo}	(13)
Human	local	Liquid	Irritating to skin and eyes	(14)
Human	contact with vapor	NS	Not irritating to the eyes and throat	(14)

* Not specified

ETHYLENE GLYCOL (cont.)

TABLE IV-1. TOXICITY OF ETHYLENE GLYCOL (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Human	inhalation	10,000 mg/m ³	TC _{Lo}	(13)
Human	inhalation	Vapors above 100°C chronic	Nystagmus and recurrent attacks of unconsciousness	(11)
Rat	oral	4,700 mg/kg	LD ₅₀	(13)
Rat	oral	0.0-1.0 g/kg/day, days 6-15 of gestation	No maternal toxicity, embryotoxicity, or increased incidence of malformations in fetuses of dosed dams	(15)
Rat	intra-peritoneal	5,220 mg/kg	LD ₅₀	(13)
Rat	intra-venous	2,800 mg/kg	LD _{Lo}	(13)
Rat	subcu-taneous	5,300 mg/kg	LD ₅₀	(13)
Rat	intra-muscular	3,300 mg/kg	LD _{Lo}	(13)
Rat	inhalation	12 mg/m ³	Corneal damage and apparent blindness without signs of systemic intoxication	(11)
Mouse	oral	7,500 mg/kg	LD ₅₀	(13)
Mouse	intra-peritoneal	5,614 mg/kg	LD ₅₀ ; chronic pulmonary edema or congestion, effects on the spleen, kidney tubules and glomeruli	(13)
Mouse	intra-venous	3,000 mg/kg	LD ₅₀	(13)
Mouse	subcu-taneous	2,700 mg/kg	LD _{Lo}	(13)
Guinea pig	oral	6,610 mg/kg	LD ₅₀	(13)
Guinea pig	subcu-taneous	5,000 mg/kg	LD _{Lo}	(13)

ETHYLENE GLYCOL (cont.)

TABLE IV-1. TOXICITY OF ETHYLENE GLYCOL (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Rabbit	intra-peritoneal	1,000 mg/kg	LD _{Lo}	(13)
Rabbit	intra-venous	5,000 mg/kg	LD _{Lo}	(13)
Rabbit	intra-muscular	5,500 mg/kg	LD _{Lo}	(13)
Rabbit	skin	19,530 mg/kg	LD ₅₀	(13)
Rabbit	skin	555 mg (open)	Moderate irritation	(13)
Rabbit	eye	100 mg/1 hr	Mild irritation	(13)
Rabbit	eye	1,440 mg/6 hr	Moderate irritation	(13)
Cat	oral	2,000 mg/kg	LD ₅₀	(13)
Cat	subcutaneous	2,000 mg/kg	LD _{Lo}	(13)

* Not specified

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF ETHYLENE GLYCOL

Test System	Dose	Effects	Reference
Human lymphocytes	320 mmol/L	DNA synthesis inhibition	(13)
Mouse lymphocytes	100 mmol/L	Mutagenic	(13)

ETHYLENE GLYCOL (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

Ala. Adsorption -- Data not available

Alb. Volatilization -- Data not available

Alc. Leachability -- The adsorption of ethylene glycol onto different soil types was studied at 6°C. No adsorption was observed onto samples of subhorizons of sandy till, clayey till, and melt water sand. Leaching experiments with undisturbed soil cores of sandy till showed that C₁₄ labelled ethylene glycol closely followed the movement of water when chloride ion was used as a water tracer (16).

Ald. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Adapted activated sludge, with ethylene glycol as sole carbon source: 96.8% removal at 41.7 mg COD/g dry inoculum/hr (6). Biooxidation of ethylene glycol was 96% in 20 days in a lightly seeded dilution-bottle test without prior acclimation of microorganisms (17). Anaerobic metabolism of ethylene glycol by culture from sludge of municipal anaerobic digester is dominated by two morphological types of bacteria, tentatively identified as a Methanobacterium sp. and a Desulfovibrio sp. Decomposition products are acetate and ethanol. Formation of methane as a product of ethanol oxidation apparently occurs only after ethylene glycol degradation is complete (18).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reactions -- BOD₅: 38% of ThOD, COD: 94% of ThOD, ThOD: 1.26

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Chimpanzees exposed to an ethylene glycol-saturated atmosphere for 28 days displayed no seriously harmful effects. Serious behavioral disturbances, such as have been observed in both man and the chimpanzee following ingestion or injection of ethylene glycol, did not occur during the periods of glycol inhalation (19).

ETHYLENE GLYCOL (cont.)

- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Toxicity threshold (cell multiplication inhibition test): bacteria >10,000 mg/L; algae = 2,000 mg/L; green algae >10,000 mg/L; protozoa >10,000 mg/L; bacteria (toxic) at 250 mg/L (6).
- B7. Aquatic species (fish and invertebrates) -- guppy: 7 day LC₅₀, 49,300 ppm (6); shrimp: 48 hour LC₅₀, greater than 100 ppm (8).

C. Effects on plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Listed in EPA TSCA Inventory 1980.

VII. DISPOSAL METHODS

AEHA: NSN 6850-00-181-7929, 7940

A. Current Recommended Army Disposal Practices (20)

- 1. Sanitary Sewer -- Ethylene glycol/water mixtures of the following strengths shall be disposed in the sanitary sewer system assuming an allowable daily increase of 25 ppm biological oxygen demand (BOD) loading for a flow of 1,000,000 gallons per day. The allowable daily increase is only applicable where the installation is meeting its National Pollution Discharge Elimination System Permit with a comfortable margin approaching 2 mg/L of BOD. The discharge shall be coordinated with treatment plant operations to ensure proper performance during discharge.

ETHYLENE GLYCOL (cont.)

TABLE VIIA-1. DISCHARGE/TREATMENT PLANT OPERATION

% Mixture (Ethylene Glycol/Water)	Gallons/l mgd for 25mg/L BOD Increase*
10	240
20	120
30	80
40	60
50	40

* Smaller allowable BOD increases will result in proportionally less waste loading.

The above material shall be metered uniformly over a 12-hour period with enough water to assure adequate flushing. An easy way to determine the percent ethylene glycol in the solution would be with an antifreeze tester and the chart given below. Thoroughly mix the antifreeze/water solution and test with the antifreeze tester; determine the percent ethylene glycol from the chart.

TABLE VIIA-2. ETHYLENE GLYCOL/TEMPERATURE (20)

% Ethylene Glycol	Temperature Protected Degrees Fahrenheit
10	+23
20	+12
30	-01
40	-24
50	-54

2. Safety and Control Measures -- Particular attention should be given to preventing skin contact. Disposal personnel should wear at least mid-arm impervious gloves and a full-length impervious apron. A faceshield and/or full face respirator approved for this item should be available if any odor is noticed during mixing or loading (20).
3. Incineration -- Do not incinerate (20).
4. Sanitary Landfill -- Do not bury (20).

ETHYLENE GLYCOL (cont.)

B. Alternative Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

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ETHYLENE GLYCOL DINITRATE

Much of the available data on ethylene glycol dinitrate has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_2H_4N_2O_6$

Molecular Weight: 152.08

Structural Formula: $O_3NCH_2CH_2NO_3$

B. Alternate Names and Registry Numbers

CAS Registry Number: 628-96-6

CA Name (9CI): 1,2-Ethanediol, dinitrate

CA Name (8CI): Ethylene glycol, dinitrate

RTECS Number: KW5600000

Other Significant Synonyms: Dinitroglycol, EGDN, ethanediol dinitrate, ethylene dinitrate

C. Chemical and Physical Properties

Physical State: Oily liquid (l)

Color: Yellow

Odor: Data not available

Melting Point: $-22.3^{\circ}C$

ETHYLENE GLYCOL DINITRATE (cont.)

Solubilities:

Water: 6.2 g/L at 15°C (2)

Nonaqueous Solvents: Soluble in ether, acetone, chloroform, benzene, nitrobenzene, and toluene. Slightly soluble in carbon tetrachloride and benzine (2).

Octanol Water Partition Coefficient: $\log P = 0.55$

Hygroscopicity: Not hygroscopic (2)

Density (Crystal): Data not available

Specific Gravity: 1.488 at 20°C (2)

Volatility: Volatile. 0.14% loss at 20°C after 24 hours; 0.37% loss after 48 hours. 100% loss after 40 days at 35°C (2).

Vapor Pressure: 0.00025 mm Hg at 20°C (1)

Specific Heat: 0.4 cal/g (2)

Heat of Combustion: 1764 kcal/kg (3)

Stability: Stable at 75°C (2)

Flammability: Ignites when contacted with flame, may explode (1).

Autoignition Temperature: 114-116°C (4). Explosive Temperature: 257°C.

II. USES

A. Army Unique Use

Liquid high explosive -- Class A explosive (4)

B. Other Uses

Used with nitroglycerin to make dynamite and other explosives. Occupational exposure involves mixing ethylene glycol dinitrate and nitroglycerin and considering the two chemicals together (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Many analytical methods have been reported recently for this compound and choice of method depends on the purpose of the analysis. Cohen et al. (6) reported an Ion Mobility Spectrometer (IMS) which can detect parts per trillion of explosive in air.

ETHYLENE GLYCOL DINITRATE (cont.)

Lloyd reported a high performance liquid chromatography method that uses a pendant mercury drop electrode at the detector. This method compares favorably with electron capture detection in gas chromatography and was developed for forensic analysis, but could be applied for other types of trace analysis (7).

Yu et al. (8) reported a method to determine this compound with nitro/nitroso specific detector with either a gas or liquid chromatograph. This method can be used in the analysis of wastewater or biological fluids. The detector is a Thermal Energy Analyzer (TEA) and can also be applied to metabolites of nitrate esters.

Cumming and Park reported a gas chromatography/single ion monitoring mass spectroscopy method (9).

B. Limit of Detection

Lloyd reported a detection limit of 2-20 picogram/10 microliters of injected sample (7).

ETHYLENE GLYCOL DINITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ETHYLENE GLYCOL DINITRATE*

Species	Route	Dose/Duration	Effects	Reference
Human	inhalation, dermal	NS**	May cause severe, throbbing headache with small exposures, and nausea, vomiting, cyanosis, coma, and death with heavier exposures	(1)
Rat	sub-cutaneous	0.5 mL/kg bw, 10% EGDN in olive oil, daily for 9 wk	Increased liver, kidney, and spleen weight to body weight ratios; increased serum glutamic oxaloacetic transaminase and acetylcholinesterase activities; methemoglobin not detected	(10)
Rat, Mouse, Guinea pig	inhalation	500-1,500 mg/m ³ for 3 wk to 3 mo	Sleepiness, Heinz body formation, anemia, increased reticulocyte count	(11)
mouse	inhalation	800 mg/m ³ , 8 hr/d, 6d/wk, for 10 wk	Lethargy, cyanosis, Heinz body formation, increased reticulocyte count, hemolytic anemia, skin erosion, thin coats, spasms; 23/30 animals dead after 24 wk	(11)
Rabbit	sub-cutaneous	1.5 mL/kg bw, 10% EGDN in olive oil, once	Increased plasma activities of lactic dehydrogenase, alkaline phosphatase, and aldolase; inhibition of plasma monoamine oxidase activity	(12)
Rabbit	sub-cutaneous	3.0 mL/kg bw, 10% EGDN in olive oil, once	Methemoglobin formation, highest levels at 2-4 hr after administration	(14)

* Information not included in the ARC report

** Not specified

ETHYLENE GLYCOL DINITRATE (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of ethylene glycol dinitrate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA: 0.05 ppm or 0.3 mg/m³; STEL: 0.1 ppm or 0.6 mg/m³ (15).

B. Environmental

Reported in TSCA Inventory 1983.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (16).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (17).

C. Other Disposal Practices Employed

Spills and leakage: Overspread sufficient sodium hydroxide and sprinkle water. Drain into the sewer with abundant water.

(a) Disposal and Waste Treatment: Dissolve in a combustible solvent such as alcohol, etc. Burn in an open furnace by igniting from a safe distance with the utmost care or sprinkle into the fire chamber of a furnace with afterburner and scrubber.

(b) Laboratory Scale Quantities: Pour into sodium bisulfate in a large evaporating dish. Sprinkle water and neutralize. Drain into the sewer with sufficient water.

ETHYLENE GLYCOL DINITRATE (cont.)

(c) Disposal Method Suggested: Controlled incineration in the scrubber equipped Deactivation Furnace incinerator (The Chemical Agent Munition Disposal System) (A-31). Also, ethylene glycol dinitrate can be recovered from wastewaters (A-58) (18).

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ETHYLENE GLYCOL MONOETHYL ETHER

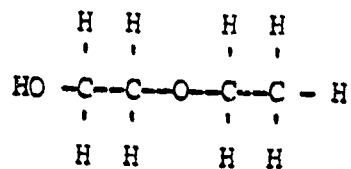
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_4H_{10}O_2$

Molecular Weight: 90.12 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 110-80-5

CA Name (9CI): Ethanol, 2-ethoxy-

CA Name (8CI): Same

RTECS Number: KK8050000

Other Significant Synonyms: ethyl cellosolve, cellosolve, ethyl 2-hydroxyethylether, Ethylethylene glycol, glycol ethyl ether, hydroxy ether, 2-ethoxyethyl alcohol, monomethyl ether of ethylene glycol

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Colorless (1)

Odor: Odorless (1)

Melting Point: $-70^{\circ}C$ (1)

Boiling Point: $135^{\circ}C$ (1)

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

Solubilities:

Water: Completely miscible (1)

Nonaqueous Solvents: Miscible with alcohol, ether, acetone and liquid esters (1).

Octanol Water Partition Coefficient: $\log P = -0.17(2); -0.54(3)$.

Hygroscopicity: Data not available

Specific Gravity: 0.931 at 20°C (1)

Volatility: Vapor density of 3 g/L (4)

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Flammable; flash point: 44°C, open cup;
49°C, closed cup(1). Autoignition temperature, 273°C (4).

II. USES

A. Army Unique Use

Solvent for nitrocellulose

B. Other Uses

Solvents for lacquers and dopes; in various removers, cleansing solutions and dye baths; finishing leather with water pigments and dye solutions; and increasing the stability of emulsions (1).

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Gas chromatography is the method of choice. Sidhu (6) reported a gas chromatography method for 2-ethoxyethanol in air. Samples were first obtained by adsorption onto activated carbon followed by desorption with carbon disulfide/isopropyl alcohol. Detection was by flame ionization detector. An FFAP column was used isothermally at 130°C. Sakai et al. (5) also used FFAP mixed with BX-10 to determine and separate paint thinner components in air, including 2-ethoxyethanol. Smallwood et al. (6) reported a gas chromatographic method of monitoring 2-ethoxyethanol in blood and its urinary metabolites by determining the pentafluorobenzyl derivatives.

B. Limit of Detection

Sidhu (6) reported 0.1 ppm as the limit of detection in air samples.

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ETHYLENE GLYCOL MONOETHYL ETHER

Species	Route	Dose/Duration	Effects	Reference
Human	ingestion	0.5-5 g/kg	Estimated lethal dose	(7)
Human	ingestion	NS*	Central nervous system depression; kidney injury; hematuria	(7)
Human	inhalation	NS*	May cause moderate irritation of the respiratory tract	(8)
Human	contact with vapor	0.6% vapor	Irritation of the eyes	(9)
Human	eye	NS*	Pain, mild irritation, and transient corneal injury	(8)
Human	skin	Prolonged or repeated exposures	Mild irritation	(8)
Test animals	inhalation	0.6% vapor for 18-24 hr	Congestion and edema of the lungs and congestion of the kidneys	(9)
Rat	oral	3,000 mg/kg	LD ₅₀	(10)
Rat	oral	1,890 mg/kg for 90 days in drinking water	Mortality	(10)
Rat	intra-peritoneal	1,200 mg/kg	LD _{Lo}	(10)

*Not specified

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

TABLE IV-2. TOXICITY OF ETHYLENE GLYCOL MONOETHYL ETHER (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Rat	intra-venous	2,400 mg/kg	LD ₅₀	(10)
Rat	inhal-ation	4,000 ppm/4 hr	LC _{Lo}	(10)
Rat, mouse rabbit	various		Teratogenic	(10)
Mouse	oral	4,300 mg/kg	LD ₅₀	(10)
Mouse	intra-peritoneal	1,707 mg/kg	LD ₅₀ ; chronic pulmonary edema or congestion, effects on kidney tubules and the spleen	(10)
Mouse	intra-venous	3,900 mg/kg	LD ₅₀	(10)
Mouse	sub-cutaneous	5,000 mg/kg	LD _{Lo}	(10)
Mouse	inhal-ation	1,820 ppm/7 hr	LC ₅₀ ; analgesia, dyspnea, hematuria	(10)
Guinea pig	oral	1,400 mg/kg	LD ₅₀	(10)
Guinea pig	eye	10 ug	Mild irritation	(10)
Guinea pig	inhal-ation	3,000 ppm/24 hr	LC _{Lo}	(10)
Rabbit	oral	3,100 mg/kg	LD ₅₀ ; anesthesia, hemolysis	(10)
Rabbit	skin	3,500 mg/kg	LD ₅₀	(10)
Rabbit	skin	500 mg (open)	Mild irritation	(10)
Rabbit	eye	50 mg	Moderate irritation	(10)
Dog	inhal-ation	840 ppm, 7 hr/day for 12 wk	Slight decrease in red cells and hemoglobin and an increase in im-mature white cells	(10)

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

Ala. Adsorption -- Data not available

Alb. Volatilization -- Data not available

lc. Leachability -- Data not available

Ald. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Bio-oxidation in 20 days with non-acclimated microbial cultures: 100% in fresh water; 62% in synthetic salt water (11).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- BOD₅: 1.58 at 5-10 ppm, normal sewage as seed material, standard dilution technique; COD: 1.92 (12); Freshwater BOD₅: 36% of theoretical, with sewage seed; Saltwater BOD₅: 5% of theoretical, with sewage seed (4); ThOD: 1.80 (11).

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

B7. Aquatic species, fish and invertebrates -- Fish: Lepomis macrochirus 96-hour LC₅₀: >10,000 ppm; Menidia beryllina 96-hour LC₅₀: >10,000 ppm; guppy, Poecilia reticulata, 7-day LC₅₀: 16,400 ppm (4); goldfish, Carassius auratus, 24-hour LC₅₀: >5,000,000 ug/L (13).

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

C. Effects on plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 5ppm (skin) (10)

B. Environmental

Reported in TSCA Inventory 1980.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (14).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (15).

C. Other Disposal Practices Employed

Spray into incinerator or burn in paper packaging. Flammable solvent may be added (4).

ETHYLENE GLYCOL MONOETHYL ETHER (cont.)

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ETHYLENE OXIDE

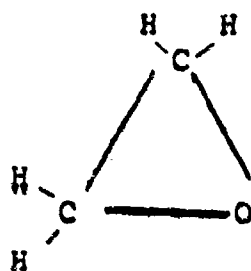
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: C_2H_4O (1)

Molecular Weight: 44.05 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 75-21-8

Deleted CAS Registry Number: 19034-08-3

CA Name (9CI): Oxirane

CA Name (8CI): Ethylene oxide

RTECS Number: KX2450000

Other significant synonyms: Dihydrooxirane, dimethylene oxide, 1,2-epoxyethane, oxycyclopropane, oxirane, dihydro-

C. Chemical and Physical Properties

Physical State: Gas at room temperature and pressure; liquid below $12^{\circ}C$.

Color: Colorless (1)

Odor: Sweet, ether-like. Minimum detectable by odor is 700 ppm (2)

Melting Point: $-111^{\circ}C$ (1)

Boiling Point: $10.7^{\circ}C$ (1)

ETHYLENE OXIDE (cont.)

Solubilities:

Water: Soluble in water (1)

Nonaqueous Solvents: Soluble in alcohol and ether (1), soluble in benzene (3).

Octanol Water Partition Coefficient: $\log = -0.3$ (4)

Hygroscopicity: Data not available

Vapor Density (Gas): 1.52 (5)

Specific Gravity (Liquid): 0.882 at 10°C (3)

Volatility: Gas at room temperature.

Vapor Pressure: 779.1 Torr at 11°C, 1,305 Torr at 25°C (6)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: May rearrange chemically and/or polymerize violently with evolution of heat on contact with catalytic surfaces (5).

Stability: Explosive (1). Do not expose to sunlight (2).

Flammability: Very flammable, flash point -18°C (1).

II. USES

A. Army Unique Use

Chemical intermediate in production of explosives.

B. Other Uses

Fumigant; sterilization of surgical instruments; agricultural fungicide; organic synthesis, especially in the production of ethylene glycol and the starting material for the manufacture of acrylonitrile and nonionic surfactants (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Gas chromatography is the method of choice. The official National Institute of Occupational Safety and Health (NIOSH) method uses activated charcoal and carbon disulfide to collect and absorb ethylene oxide (ETO) onto a gas chromatography with a flame ionization detector. Esposito et al. (6) reported a U.S. Army Environmental Hygiene Agency (USAEHA) gas chromatography method using a chemically impregnated

ETHYLENE OXIDE (cont.)

sampling tube to collect the ETO before chromatography. Ambersorb 347 was treated with HBr and placed in air sampling tubes. Air was drawn through the tubes where ETO was converted to 2-bromoethanol. The tubes are desorbed with a mixture of acetonitrile and toluene and chromatographed on diethylene glycol succinate on Chromosorb WHP column with an electron capture detector (ECD).

B. Limit of Detection

Esposito et al. reported 0.5 ppm (6).

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ETHYLENE OXIDE

Species	Route	Dose/Duration	Effects	Reference
Human	oral	50-500 mg/kg	Estimated lethal dose	(7)
Human, animals	skin, inhalation, ingestion	Acute	Primary irritation or burns of skin, eyes, lungs, and respiratory tract; skin sensitization; vomiting; diarrhea	(8)
Human, animals	eye	Liquid or vapor	Severely irritating	(8)
Human, animals	skin, inhalation	Min dose: 1 ppm avg. exposure for 15 yr	Potential adverse effects on lungs, liver, kidneys, adrenal glands, testes, blood, and the central nervous system	(8)
Human, rat, rabbit, monkey	inhalation	Min. dose: 204 ppm repeated exp. for 176 days	Evidence of reversible peripheral neuropathy	(8)
Human	occupational exposure	4-10 yr	Increased rate of leukemia	(9)
Human	inhalation	12,500 ppm, 10 sec	TC _{Lo} ; effects on sense organs	(10)
Human	inhalation	500 ppm, 2 min	TC _{Lo} ; convulsions, nausea, respiratory	(10)

ETHYLENE OXIDE (cont.)

			changes	
Rat	oral	30 or 7.5 mg/kg 2x/wk for up to 150 wk	Squamous-cell carcinomas of the forestomach; hyperkeratosis, hyper- plasia, papillomas of the stomach squamous epi- thelium	(11)
Rat	oral	72-330 mg/kg	LD ₅₀	(10,8)

TABLE IV-1. TOXICITY OF ETHYLENE OXIDE (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Rat	inhal- ation	1,462 ppm, 4 hr	LC ₅₀ ; lacrimation, salivation, diarrhea	(10)
Rat, mouse	various		Teratogenic	(10)
Rat	inhal- ation	0, 50, or 100 ppm for 104 wk	Increased incidences of mononuclear cell leuke- mia, peritoneal mesothe- lioma, and mixed cell brain glioma	(10)
Rat, mouse guinea pig	inhal- ation	Min. dose: 1.98 ppm for 66 days	Testicular atrophy; dominant lethal effects	(8)
Mouse	intra- peritoneal	100 mg/kg	LD _{Lo}	(10)
Mouse	intra- venous	290 mg/kg	LD ₅₀	(10)
Mouse	sub- cutaneous	292-2,576 mg/kg, total dose, inter- mittently for 95 wk	Lymphomas and injection- site tumors	(10)
Mouse	inhal- ation	836 ppm, 4 hr	LC ₅₀	(10)
Guinea pig	oral	270 mg/kg	LD ₅₀	(10)
Guinea pig	inhal- ation	7,000 ppm, 150 min	LC _{Lo}	(10)

ETHYLENE OXIDE (cont.)

Rabbit	eye	18 mg, 6 hr	Moderate irritation	(10)
Rabbit	intra-venous	175 mg/kg	LD _{Lo}	(10)
Dog	intra-venous	125 mg/kg	LD ₅₀	(10)
Dog	inhal-ation	960 ppm, 4 hr	LC ₅₀ ; lacrimation, nausea, diarrhea	(10)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF ETHYLENE OXIDE

Test System	Effects	Reference
Bacteria, <u>Drosophila melanogaster</u> , mammalian cells <u>in vitro</u> , mammals <u>in vivo</u>	Produces mutagenicity and related effects in many test systems	(10)
Human	Chromosomal aberrations in workers accidentally exposed to ethylene oxide at approx. 1,500 ppm for 2 hr	(8)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

Al. Transport

Ala. Adsorption -- Data not available

Alb. Volatilization -- The desorption rate of ethylene oxide from natural waters is about 0.36 times that of oxygen under the same conditions (12).

Alc. Leachability -- Data not available

Ald. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Possible metabolites include ethylene glycol, ethylene chlorohydrin and glyoxal. Biooxidation of ethylene oxide proceeds at rates indicating nonpersistence. In a lightly seeded BOD test, 52% of ethylene oxide was oxidized in 20 days without prior

ETHYLENE OXIDE (cont.)

acclimation. In a biological waste treatment system with a high concentration of adapted microorganisms, biooxidation would be much faster, perhaps a matter of hours (12).

- A2b. Hydrolysis -- In fresh water ethylene oxide hydrolyzes to ethylene glycol. In salt water systems, ethylene chlorohydrin is also formed; the ratio of chlorohydrin to glycol formed is directly proportional to the salt concentration (about 0.2 at 3% NaCl) (12).
- A2c. Photolysis -- Degrades in atmosphere by free radical processes; intermediate radicals include $\text{CH}_3\cdot$ and HCO or $\text{H} + \text{CO}_2$ (13).
- A2d. Other Chemical Reaction -- Data not available
- A2e. Half-life -- The hydrolysis half-life of ethylene oxide is about 14 days in fresh water at 25°C . Temperature effects are greater than pH effects at pH levels usually encountered. The hydrolysis/hydrochlorination half-life of ethylene oxide in salt water is about 9 days at 25°C (12).

B. Effects on Animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- The adverse effect level of ethylene oxide on activated sludge microorganisms or the LC_{50} (concentration that inhibited growth 50%) was determined to be in the range of 10 to 100 mg/L (12).
- B7. Aquatic species, fish and invertebrates -- 96-hour LC_{50} for fathead minnow: 84 mg/L, 48-hour LC_{50} for Daphnia magna: 212 mg/L, 48-hour LC_{50} for brine shrimp: 745 mg/L (12).

C. Effects on Plants

- C1. Phytotoxicity -- One percent aqueous extracts of manure, activated sludge and digested sludge, stored for 2, 26, 27 or 65 days, inhibited seed germination and root growth in Brassica parachinensis. Inhibition appeared to be associated with high levels of ammonia, and to a lesser extent, ethylene oxide (14).
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

ETHYLENE OXIDE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in TSCA Inventory 1983.

EPA TSCA 8(a) Preliminary Assessment Information, final rule (15).

Ethylene oxide has a statutory reportable quantity (RQ) of 1 lb under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (16).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Data not available

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Dissolve in higher alcohol, benzene, or petroleum ether. Incinerate.

Ether of long standing may contain peroxides. Transport to isolated area in padded containers. Uncover and arrange excelsior train. From distance, puncture with rifle fire and ignite excelsior (5).

AEHA: NSN 6505-00-C99-3878, 3962, 3405, 5298

Dispose of through a commercial contractor (17).

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HALAZONE

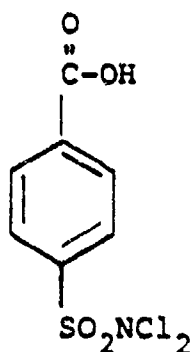
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_7H_5Cl_2NO_4S$

Molecular Weight: 270.09

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 80-13-7

CA Name (9CI): Benzoic acid, 4-[(dichloroamino)sulfonyl]

CA Name (8CI): Benzoic acid, p-(dichlorosulfamoyl)

RTECS Number: DG8050000

Other Significant Synonyms: Carboxybenzenesulfonedichloroamide; p-N,N-dichlorosulfamyl benzoic acid; p-sulfonedichloramidobenzoic acid.

C. Chemical and Physical Properties

Physical State: Crystalline powder (1)

Color: White (1)

Odor: Strong chlorine odor

Melting Point: 195°C (decomposition) (1)

HALAZONE (cont.)

Solubilities:

Water: slightly (1)

Nonaqueous Solvents: soluble in glacial acetic acid, benzene;
slightly soluble in chloroform; insoluble in petroleum ether (1).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Field water treatment

B. Other Uses

Water disinfectant (1)

III. ANALYTICAL METHODS

A. Best Acceptable Method

No appropriate methods were found for trace analysis of this compound.

B. Limit of Detection

Data not available

HALAZONE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF HALAZONE

Species	Route	Dose/Duration	Effects	Reference
Rat	oral	3,500 mg/kg	LD ₅₀	(2)
Rat	intra venous	300 mg/kg	LD _{Lo}	(2)

V. ENVIRONMENTAL EFFECTS

This material releases free chlorine on reaction with water. While little information on specific environmental fate of halazone is available, the compound is believed to have effects similar to that of high levels of free chlorine.

A. Environmental Fate

A1. Transport -- Data not available

A2. Transformation -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Halazone was found to have a considerable disinfecting action in river water. Doses ranging from 1.0 to 50.0 mg/L of halazone reduced bacterial counts, on average, by 73.31% to 99.41% after 48 hours' incubation. At doses of less than 1.0 mg/L the bacterial count generally increased (3).

B7. Aquatic species, fish and invertebrates -- Data not available

C. Effects on plants -- Data not available

HALAZONE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for Water Purification Kit (the principal use of halazone) is burial in a sanitary landfill (4).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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HYDRAZINE

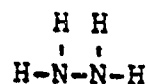
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: N_2H_4

Molecular Weight: 32.06

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 302-02-2

CA Name (9CI): Hydrazine

CA Name (8CI): Hydrazine

RTECS Number: MU7175000

Other Significant Synonyms: Diamine

C. Chemical and Physical Properties

Physical State: Fuming, colorless, hygroscopic, liquid (1) or white crystals (2)

Color: Colorless

Odor: Penetrating, resembling that of ammonia (3)

Odor Index: 5,300 at 20°C (4)

Threshold Odor Concentration: 3-4 ppm (4)

Melting Point: 2.0°C (3)

Boiling Point: 113.5°C (3)

HYDRAZINE (cont.)

Solubilities:

Water: Miscible with water (3).

Nonaqueous Solvents: Miscible with methyl, ethyl, propyl, and isobutyl alcohols (3). Slightly miscible with hydrocarbons and halogenated hydrocarbons (5). Insoluble in chloroform and ether (1).

Octanol Water Partition Coefficient: $\log P = -1.11$ (6)

Hygroscopicity: Hygroscopic: readily forms hydrate, $N_2H_4 \cdot H_2O$ (7)

Specific Gravity: 1.0083 at 4°C (5)

Volatility: Data not available

Vapor Pressure: 10.4 mm Hg at 20°C (8)

Flash Point: 38-52°C (Open cup) (8)

Saturation Concentration: 18,900 ppm at 25°C (8)

Refractive Index: n (35°C) 1.4644 (5)

Autoignition Temperature: 24°C, iron-rust surface; 270°C glass surface (8).

Heat of Combustion: 148.6 cal/mol (1)

Reactivity: Explosion hazard when exposed to heat or flame or by chemical reaction with alkali metals, NH_3 , Cl_2 , chromates, CuO , Cu^{++} salts, F_2 , H_2O_2 , iron rust, metallic oxides, Ni , $Ni(ClO_4)_2$, HNO_3 , N_2O , O_2 , $K_2Cr_2O_7$, $Na_2Cr_2O_7$, tetryl, zinc, diazide, and $Zn(C_2H_5)_2$ (2). Explodes during distillation if traces of air are present; also affected by UV. Strong reducing agent, diacidic base ($pK_B=5.52$) (3).

Stability: Thermodynamically unstable and may decompose to hydrogen, ammonia and nitrogen; the reaction rate is reportedly slow at room temperature but is rapid at elevated temperatures, particularly in the presence of metals such as copper (8). If air is excluded, hydrazine can be stored, preferably in the form of the hydrate, without decomposition for a long time in paraffin bottles (5). Can be stored sealed in glass and kept in a cool, dark place (3). Usually stored under nitrogen (9).

Flammability: Fire hazard dangerous, when exposed to heat, flame or oxidizing agents (2). Combustion highly exothermic (1).

Flammable limits: 4.7-100% by volume in air, combustion produces toxic vapor (10).

HYDRAZINE (cont.)

II. USES

A. Army Unique Use

Propellant

B. Other Uses

Hydrazine is used as a polymerization catalyst, blowing agent, reducing agent, oxygen scavenger, and short-stopping agent. Other uses include Spandex fibers, explosives, antioxidants (petroleum, detergents), plating metals on glass and plastics, fuel cells, solder fluxes, scavenger for gases, photographic developers, corrosion inhibitors, oil-well drilling in soils containing kaolinite, buoyancy agent for undersea salvage, diving equipment, boiler feedwater, and reactor cooling water. Hydrazine is used in the synthesis of agricultural chemical (maleic hydrazide) and the manufacture of pharmaceuticals (antibacterial and antihypertensive agents) (1).

III. ANALYTICAL METHODS

Hydrazine can be determined by titration, colorimetry, potentiometry, or gas chromatography. Small quantities (less than 1 ppm) can be determined photometrically after reaction with p-dimethylaminobenzaldehyde to yield an intense red color with a minimum transmittance at 445 nm or 455 nm (6).

A. Best Acceptable Method

For the analysis of hydrazine, methylhydrazine, 1,1-dimethylhydrazine, and phenylhydrazine in workroom air, the National Institute of Occupational Safety and Health (NIOSH) (8) recommends the Wood-Anderson gas chromatographic method because of its high sensitivity and specificity. With this method, air samples are collected in a sulfuric acid-coated silica gel sorbent and the hydrazinium hydrogen sulfates are desorbed from the gel with water. The resulting solution is neutralized with sodium acetate and reacted with 2-furaldehyde. The derivatives formed are extracted into ethyl acetate and determined by gas chromatography with flame ionization detection.

Recently, two rapid methods easily adapted for field monitoring, have been reported. Holtzclaw et al. (11) reported a simplified trapping system using a chilled acetone collection medium, where a stable derivative of hydrazine is formed. The acetone solution can then be directly injected into a gas chromatograph equipped with thermionic and a TEA nitrogen analyzer (11). Anderson et al. reported a high pressure liquid chromatographic method using chemisorption tubes containing benzaldehyde-coated XAD-2 resin (12).

HYDRAZINE (cont.)

B. Limit of detection

4 ppb (11)

5 ug/m³ (12)

IV. HEALTH EFFECTS

TABLE IV-1. ACUTE TOXICITY OF HYDRAZINE* (13)

Species	Route	LD ₅₀ or LC ₅₀
Rat	oral	60 mg/kg
Rat	ip	59 mg/kg
Rat	iv	55 mg/kg
Rat	inh	570 ppm/4hr
Mouse	oral	59 mg/kg
Mouse	ip	62 mg/kg
Mouse	iv	57 mg/kg
Mouse	inh	252 ppm/4hr
Mouse	unknown	200 mg/kg
Guinea pig	skin	190 mg/kg**
Rabbit	iv	20 mg/kg
Rabbit	skin	91 mg/kg
Dog	iv	25 mg/kg

*Data from RTECS (1984) except **from NIOSH (8)

HYDRAZINE (cont.)

TABLE IV-2. TOXIC EFFECTS OF HYDRAZINE

Species	Route	Dose/Duration	Effects	Reference
Human	inhalation	NS	Eye and upper respiratory sensitization-type dermatitis, eye and skin burns, lethargy, tremors, vomiting, diarrhea	(9)
Rat	inhalation	20-225 ppm, 6 hr/d, 5 d/wk, x6 wk	Death of 83% in 1-6 wk	(8)
Rat	inhalation	5-14 ppm, 6 hr/d, 5 d/wk, x6 mo	Some deaths	(8)
Dog	intravenous	25-100 mg/kg single dose	Hypoglycemia, convulsions	(8)
Dog	intravenous	16-20 mg/kg single dose	Impaired kidney function	(8)
Dog	subcutaneous	16-25 mg/kg single dose	Elevated plasma ammonia levels without significant elevation of blood urea nitrogen	(14)
Dog	inhalation	150-168 ppm-hr/wk x6 mo	Weight loss, fatty liver, anemia	(8)
Dog	inhalation	14 ppm, 6 hr/d, 5 d/wk, x6 mo	Fatty liver, anemia, death in 2 of 4	(8)
Dog	inhalation	5 ppm, 6 hr/d, 5 d/wk, x6 mo	Weight loss, vomiting, irregular breathing	(8)
Rhesus monkey	intraperitoneal	5-20 mg/kg, 25-33 doses	Weight loss, slight anemia, fatty liver, kidney, and heart	(8)
Rhesus monkey	intraperitoneal	32 mg/kg, 2 doses	Inhibition of insulin release	(8)

HYDRAZINE (cont.)

TABLE IV-3. TERATOGENIC/REPRODUCTIVE EFFECTS OF HYDRAZINE* (13)

Species	Route	Duration	TD _{Lo} or TC _{Lo}	Effects
Rat	intra-peritoneal	Gestation days 6-15	100 mg/kg	Effects on fertility
Rat	intra-peritoneal	Gestation days 6-15	50 mg/kg	Embryotoxicity
Rat	intra-peritoneal	Gestation days 7-9	30 mg/kg	Developmental abnormalities, effects on fertility, embryotoxicity
Rat	subcutaneous	Gestation days 1-20	80 mg/kg	Embryotoxicity, newborn effects
Rat	skin	Gestation day 9	50 mg/kg	Effects on fertility
Rat	inhalation	Gestation days 1-11	1 mg/m ³ /24 hr	Embryotoxicity
Mouse	intra-peritoneal	Gestation days 6-9	48 mg/kg	Developmental abnormalities, embryotoxicity
Mouse	intra-peritoneal	Gestation days 6-9	80 mg/kg	Developmental abnormalities

HYDRAZINE (cont.)

TABLE IV-4. CARCINOGENICITY OF HYDRAZINE* (13)

Species	Route	Duration	TD _{Lo} or TC _{Lo}	Effects
Rat	inhal- ation	6 hr, 1 yr intermittently	1 ppm	Equivocal evidence for nasal tumors
Mouse	oral	2 yr, contin- uously	1951 mg/kg	Neoplastic effects: pulmonary system, blood
Mouse	intra- peri- toneal	5 wk, intermit- tently	400 mg/kg	Carcinogenic effects: blood
Mouse	inhal- ation	6 hr, 1 yr intermittently	1 ppm	Equivocal evidence for nasal tumors
Hamster	inhal- ation	6 hr, 1 yr, intermittently	5 ppm	Equivocal evidence for nasal tumors

TABLE IV-5. MUTAGENICITY AND RELATED EFFECTS OF HYDRAZINE* (13)

Test System	Dose	Effects
<u>E. coli</u>	10 μ mol/L	DNA damage
<u>S. typhimurium</u>	12 μ g/L	Microsomal-mediated mutation
<u>B. subtilis</u>	10 mmol/L	Not specified
<u>X. influenzae</u>	2 mmol/L	Mutation
<u>D. melanogaster</u>	20 mmol/L(oral)	Specific locus mutation
<u>D. melanogaster</u>	10 mmol/L(oral)	Nondisjunction
<u>S. cerevisiae</u>	200 mmol/L	Mutation
Human liver cells	80 μ g/L	Oncogenic transformation
Rat liver cells	3 mmol/L	DNA damage
Rat lung cells	250 μ g/L	Unscheduled DNA synthesis
Mouse lymphocytes	1 mmol/L	Mutation
Mouse host-mediated assay with <u>S.</u> <u>typhimurium</u>	3100 μ g/kg	Mutation
Hamster kidney cells	80 μ g/L	Oncogenic transformation
Hamster ovary cells	250 μ g/L	Unscheduled DNA synthesis
Hamster lung cells	250 μ g/L	Unscheduled DNA synthesis
Hamster ovary cells	1 mmol/L	Sister chromatid exchange
Hamster lung cells	1 mmol/L	Sister chromatid exchange

*Data from RTECE

HYDRAZINE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

Al. Transport

Ala. Adsorption -- Data not available

Alb. Volatilization -- MacNaughton et al. reports that hydrazine evaporation rates from liquid pools ranged from 16 to 100 mg/cm²/hr. These rates were considered sufficient to generate hazardous atmospheric concentrations (greater than 3 ppm) up to 2 km downwind under worst-case meteorological conditions, following release of hydrazine into the environment. Hydrazine evaporation decreases as a function of time due to absorption of H₂O and CO₂ (15).

Alc. Leachability -- Data not available

Ald. Bioaccumulation -- None of the hydrazines on which metabolic studies have been conducted seem to preferentially concentrate the chemicals or metabolites in specific organs (16). Hydrazine does not concentrate in the food chain (11).

A2. Transformation -- Data not available

A2a. Biodegradation -- About 50% of hydrazine administered to laboratory mammals has been observed to be excreted unchanged in the urine (16). Hydrazine is co-metabolized to nitrogen gas by Nitrosomonas with the major product being nitrogen (17).

A2b. Hydrolysis -- Decomposition slow in water at room temperature (9). (See A2e). Degradation in fresh or saline water is rather slow; therefore, degradation will not be a significant sink for hydrazine in aqueous environments, and downstream concentration of hydrazine will be a function of dilution and dispersion (15).

A2c. Photolysis -- Hydrazine does not photolyze in the solar actinic region ($\lambda > 290$ nm) (18).

A2d. Other chemical reaction -- Based on simulated atmosphere studies, consumption by ozone and hydroxyl radicals is expected to dominate the fate of hydrazine in the atmosphere. The half-life for the reaction of hydrazine with ozone is expected to range from less than 10 minutes in ozone pollution to less than 2 hours in the natural atmosphere; the major reaction product is hydrogen peroxide. For reactions with OH[•], the tropospheric half-life for hydrazine should range from less than one hour in polluted urban atmospheres to 3 to 6 hours in unpolluted atmospheres. Due to the apparent efficient conversion of hydrazine nitrogen to N₂, hydrazine release should have

HYDRAZINE (cont.)

relatively little impact on the levels of NO_x , nitrates, or other forms of active nitrogen in the atmosphere (18). Hydrazine degradation was faster in hard water than in soft water samples and also in relatively polluted samples which were rich in organic matter (19).

A2e. Half-life

In air, at 25°C: approximately 6 hours; in oxygenated aqueous solutions (pond and sea water): 5 days (15).

B. Effects on Animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Adequate studies in different species of laboratory mice have demonstrated that hydrazine given mainly as the hydrazine sulphate (HS) produces a high incidence of multiple pulmonary adenomas and adenocarcinomas (6).

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- The teratogenic effect of hydrazine on embryos of toad (20) and frog (17) was 10 mg/L and 40 mg/L, respectively.

B6. Microorganisms, aquatic and soil -- EC_{50} values (concentrations necessary to reduce substrate metabolism by 50%): Nitrobacter 14.6 mg/L; Nitrosomonas 94.8 mg/L denitrifying bacteria 65 mg/L anaerobic bacteria 145 mg/L (17). At a concentration of 48 mg/L, hydrazine produced a 75% inhibition of the nitrification process of non-acclimated activated sludge (5).

B7. Aquatic species, fish and invertebrates -- For Daphnia, LC_{50} = 1.2 mg/L. For several species of fish, the 24-hour LD_{50} was about or less than 4mg/L (17). Perturbation of trout was detected at 0.7 mg/L after 24-hour exposure, and a concentration of 146 mg/L was fatal to rainbow trout after 22 minutes exposure (5). Fertilized eggs of fathead minnow Pimephales promelas were exposed to hydrazine for 48 hours at various concentrations; 5 mg/L was lethal and 1.0 mg/L caused such deformation that the larvae which did hatch had little chance of survival. For bluegill, Lepomis macrochirus, 96 hour LC_{50} = 1080 mg/L (21)

C. Effects on Plants

C1. Phytotoxicity -- Hydrazine is mutagenic in higher plants (22).

HYDRAZINE (cont.)

- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

TWA 0.04 mg/m³ (0.03 mg/L, free base) (9).

B. Environmental

TLV 1 ppm (1.3 mg/m³), 1974 (5).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), who have the responsibility to review current disposal practices and to develop plans for future disposal practices (23).

B. Alternate Disposal Practices Under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot and Hawthorne Naval Ammunition Depot (24).

C. Other Disposal Practices Employed

(a) Dilute with water to produce a 40% solution. Neutralize with sulfuric acid. Drain into the sewer with abundant water (25).

(b) Dissolve in a combustible solvent (alcohols, benzene, etc.). Burn in an open pit with utmost care. Ignite from a safe distance (25).

Lunn and Sansone report a one-step approach to conversion of hydrazines to innocuous products in laboratory wastes or in the environment, using one of two nickel-based catalytic reduction procedures (26).

HYDRAZINE (cont.)

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HYDROXYL AMMONIUM NITRATE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{N}_2\text{H}_4\text{O}_4$

Molecular Weight: 96.04 (1)

Structural Formula: $\text{HONH}_3^{+1} \text{NO}_3^{-1}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 13465-08-2

CA Name (9CI): Hydroxylamine, nitrate (salt)

CA Name (8CI): Same

RTECS Number: Data not available

Other Significant Synonyms: Hydroxylamine mono nitrate

C. Chemical and Physical Properties

Physical State: Crystal (1)

Color: White (1)

Odor: Data not available

Melting Point: 48°C (1)

Solubilities:

Water: Very soluble (cold); decomposes (hot) (1).

Nonaqueous Solvents: Very soluble in alcohol (1)

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

HYDROXYL AMMONIUM NITRATE (cont.)

Heat of Combustion: Data not available

Reactivity: Reacts with inorganic and organic soil components. (2)

Stability: Decomposes at 100°C (1). Unstable in water (2).

Flammability: Data not available

II. USES

A. Army Unique Use

Propellant

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

Kaplan et al. (2) determined hydroxylammonium nitrate by spectrophotometer at 705 nm. The aqueous solutions were 50 ppm and below. No separation was performed.

B. Limit of Detection

Data not available

HYDROXYL AMMONIUM NITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF HYDROXYLAMMONIUM NITRATE

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Hydroxyl- ammonium nitrate (grade not specified)	Rat	oral	882 mg/kg	LD ₅₀	(3)
	Rat, rabbit	NS*	NS	Cyanosis, respiratory distress, and convul- sions	(3)
	Rabbit	oral	100 mg/kg	Approximate lethal dose	(3)
	Rabbit	dermal (unoc- cluded)	70 mg/kg	LD ₅₀	(3)
Hydroxyl- ammonium nitrate (technical grade; 80% aqueous solution)	Rabbit	dermal (nonoc- clusive patch)	5 d/wk for 3 wk: 0.7-11.7 mg/kg	Chronic and ulcerative dermatitis	(3)
			1.5-11.7 mg/kg	Red blood cell de- struction and Heinz body formation	
			2.9-11.7 mg/kg	Splenic hematopoiesis; increased spleen-to- body weight ratio	
			5.9-11.7 mg/kg	Hepatic hematopoiesis	
			11.7 mg/kg	Increased heart-to- body weight ratio	
Nitrates	Human	oral	Large amounts	Dizziness, abdominal cramps, vomiting, bloody diarrhea, weak- ness, convulsions, and collapse	(4)
			Small repeated doses	May lead to weakness, general depression, headache, and mental impairment	

HYDROXYL AMMONIUM NITRATE (cont.)

TABLE IV-1. TOXICITY OF HYDROXYLAMMONIUM NITRATE (Cont.)

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Hydroxyl- amine	Rat	intra- venous	59 mg/kg	LD ₅₀	(5)
	Rat	subcu- taneous	29 mg/kg	LD ₅₀	(5)
	Mouse	intra- perito- neal	60 mg/kg	LD ₅₀	(5)
	Mouse	unknown	175 mg/kg	LD ₅₀	(5)
	NS	local	NS	A moderate irritant to skin, eyes, and mucous membranes	(4)
	NS	sys- temic	NS	Can cause methemoglo- binemia	(4)

* Not specified

HYDROXYL AMMONIUM NITRATE (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF HYDROXYLAMINE⁽⁵⁾

Test System	Dose	Effects
<u>Salmonella typhimurium</u>	5 pph	Mutation; effects on DNA repair
<u>Escherichia coli</u>	5 pph	Mutation
<u>E. coli</u>	50 mmol/L	DNA damage
<u>Bacillus subtilis</u>	1 mol/L	Mutation
<u>B. subtilis</u>	100 mmol/L	DNA damage
<u>Haemophilus influenzae</u>	140 mmol/L	Mutation
	5 min	
Microorganisms	10-1,000 mmol/L	Mutation
Microorganisms	1 mol/L	Unscheduled DNA synthesis
<u>Drosophila melanogaster</u>	30 mmol/L	Sex chromosome loss and nondisjunction
<u>Neurospora crassa</u>	1 mol/L	Mutation
<u>Schizosaccharomyces pombe</u>	1 mol/L	Mutation
Human lymphocytes	360 umol/L	DNA synthesis inhibition
Human fibroblasts	300 umol/L	Chromosomal aberrations
Human leucocytes	25 mg/L	Chromosomal aberrations
Mouse embryo cells	50 umol/L	Chromosomal aberrations
Hamster lung cells	5 mmol/L	Sister chromosome exchange
Hamster ovary cells	150 mg/L/ 16 hr	Mutation
Monkey kidney cells	25 mg/L	Chromosomal aberrations
Monkey kidney cells	50 mg/L	Induction of micronuclei

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

- A1. Transport -- Data not available
- A1a. Adsorption -- Data not available
- A1b. Volatilization -- Data not available
- A1c. Leachability -- Data not available
- A1d. Bioaccumulation -- Data not available
- A2. Transformation -- Data not available

HYDROXYL AMMONIUM NITRATE (cont.)

- A2a. Biodegradation -- Data not available
- A2b. Hydrolysis -- Hydroxylammonium nitrate was stable at pH 4.9 and below.
The compound was found to be chemically unstable above a pH of about 5.9 (2).
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Reports in the literature indicate that hydroxylamine rapidly disappears from soils through a number of chemical reactions with inorganic and organic soil components (2).
- A2e. Half-life -- Data not available
- B. Effects on animals
 - B1. Avian species -- Data not available
 - B2. Mammalian wildlife species -- Data not available
 - B3. Terrestrial invertebrates -- Data not available
 - B4. Reptiles -- Data not available
 - B5. Amphibians -- Data not available
 - B6. Microorganisms, aquatic and soil -- Data not available
 - B7. Aquatic species, fish and invertebrates -- Data not available
- C. Effects on plants
 - C1. Phytotoxicity -- Data not available
 - C2. Uptake -- Data not available
 - C3. Metabolism -- Data not available
- VI. STANDARDS AND REGULATIONS
 - A. Health -- Data not available
 - B. Environmental
Reported in EPA TSCA Inventory.

HYDROXYL AMMONIUM NITRATE (cont.)

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (6).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (7).

C. Other Disposal Practices Employed

Data not available

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HYDROXYL AMMONIUM NITRATE (cont.)

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LEAD AZIDE

SUMMARY OF PREVIOUS STUDY

The Army's need for research on the toxicological and environmental hazards of lead azide was reported in A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals by the Atlantic Research Corporation (ARC). Specific data on the toxicity or environmental effects of lead azide were not reported. It was concluded, however, that lead azide is toxic to man, based on the toxicities of both lead and the azide ions, hydrazoic acid. Toxicity to aquatic organisms was expected to be low due to the insolubility of lead azide in water. The report concluded that the compound will accumulate in sediments. Some information was provided on the phytotoxicity and effects on microorganisms of other insoluble lead compounds, which may be related to the environmental effects of lead azide. The report documented that before the Army disposes of lead azide, it is treated with either sodium hydroxide or sodium nitrite and acetic acid to eliminate the explosion hazard. Thus, little if any lead azide enters the environment (1).

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: PbN_6

Molecular Weight: 291.25

Structural Formula: $\text{Pb}^{+2} (\text{N}=\text{N}=\text{N})_2^{-1}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 13424-46-9

CA Name (9CI): Lead Azide, $\text{Pb}(\text{N}_3)_2$

CA Name (8CI): Lead Azide, $\text{Pb}(\text{N}_3)_2$

RTECS Number: OF8670000

Other Significant Synonyms: Initiating explosive, lead azide

C. Chemical and Physical Properties

Physical state: Crystalline solid; alpha form is orthorhombic, beta form is monoclinic. Beta form slowly converts to alpha form at 160°C (2).

Color: Colorless

Odor: Data not available

LEAD AZIDE (cont.)

Melting Point: 245-250°C - decomposes when heated slowly

Solubility: Insoluble in aqueous ammonia; 0.125 g in 100 mL of concentrated sodium nitrate at 18°C; 0.487 g/100mL at 80°C 1.542 g per 100 mL of concentrated sodium acetate; 2.020 g per 100 mL at 80°C (2).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: 90% Rh and 30°C

Density: 4.71 g/cc alpha form; 4.93 g/cc beta form (2).

Volatility: Data not available

Vapor Pressure: Data not available

Specific heat: 0.110 cal/g at -50 to 50°C; 0.100 cal/g at 100°C (1).

Heat of Combustion: 630 kcal/kg (3)

Reactivity: Violent reaction with brass, explosion hazard severe when shocked or exposed to heat or flame. Detonates at 350°C (4).

Stability: Decomposes slowly by ultraviolet light (1). Should always be handled under water. Explosions have occurred where azide compounds have reacted with Pb in plumbing after being washed down a sink (4).

Flammability: Data not available

II. USES

A. Army Unique Use

Initiating explosive in detonators, priming compositions, and commercial blasting caps.

B. Other Uses

Primary detonator for high explosives. Information storage on styrene-butadiene resins, preparation of electrophotographic layers.

III. ANALYTICAL METHODS

A. Best Acceptable Method

Forensic scientists are currently using X-ray photoelectron spectroscopic (XPS) detection for this compound in explosive residues (5). Differential pulse polarography is used for analysis for specifications (6), but not for trace analysis. Asplund (7) reported a voltammetric method of determination that can be used for both quality

LEAD AZIDE (cont.)

control and trace environmental samples. Trace analysis was reported for azide as the sodium azide. Boehm (8) reported a TLC (thin-layer chromatography) method.

B. Limit of Detection

Sharma reports ng/cc for XPS (5).

Asplund (7) reports 0.05 mg per cubic meter of air as the sodium azide.

IV. HEALTH EFFECTS

No information updating that in the ARC report was located.

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of lead azide which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 0.15 mg (Pb)/m³; STEL 0.45 mg(Pb)/m³ (9).

The Occupational Safety and Health Administration standard - airborne, 8-hour TWA is 50 ug(Pb)/m³.

B. Environmental

Reported in the EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Data not available

B. Alternate Disposal Practices Under Consideration by the Army

A method for disposal of large quantities of lead azide by electrolytic decomposition has recently been developed and has been implemented at Savannah Army Depot. In this technique, lead azide is dissolved in the electrolyte NaOH; lead is plated out on the cathode and nitrogen is released at the anode (10).

LEAD AZIDE (cont.)

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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LEAD STYPHNATE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_3N_3O_8 \cdot Pb$ (1)

Molecular Weight: Anhydrous 450.30; monohydrate 468.3 (1)

Structural formula: See Exhibits 34-1, 34-2 and 34-3.

B. Alternate Names and Registry Numbers

CAS Registry Number: 15245-44-0

Deleted CAS Registry Numbers: 59286-40-7; 4219-19-6

CA Name (9CI): 1,3-Benzenediol, 2,4,6-trinitro-, lead(2+) salt (1:1)

CA Name (8CI): Resorcinol, 2,4,6-trinitro-, lead (2+) salt (1:1)

RTECS Number: OG6425000

Other significant synonyms: Initiating explosive lead styphnate, lead tricininate; lead trinitroresorcinate (2).

C. Chemical and Physical Properties

Physical State: Monoclinic crystals

Color: Orange-yellow

Odor: Data not available

Melting Point: Data not available

Boiling Point: Data not available

Solubilities: Data not available

Water: Very slightly soluble in water (0.04% at room temperature)(1)

Nonaqueous Solvents: Insoluble in ether, chloroform, CCl_4 , HCl.

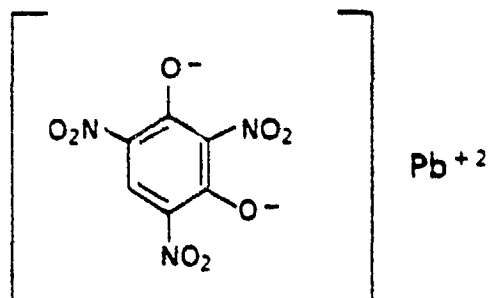
Slightly soluble in 10% aqueous ammonia acetate. Decomposed by concentrated nitric or sulfuric acid (1).

Octanol Water Partition Coefficient: Data not available

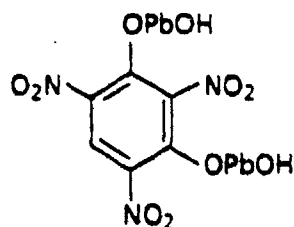
Hygroscopicity: Data not available

LEAD STYPHNATE (cont.)

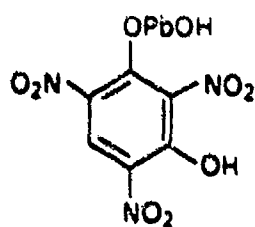
EXHIBIT 34-1



Lead styphnate compound I: lead trinitroresorcinate



Lead styphnate compound II: Dibasic lead styphnate



Lead styphnate compound III: Monobasic lead styphnate

LEAD STYPHNATE (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: 1251 kcal/kg (1)

Reactivity: Data not available

Stability: Very sensitive explosive. Shock-sensitive, has detonated when dry (1).

Flammability: Easily ignited by flame or electric spark (1).

II. USES

A. Army Unique Use

Primer initiating explosive (1)

B. Other Uses

A weak primary explosive, used in non-corrosive ignition cups such as Sinoxyd. It is added to lead azide detonators to facilitate ignition and is used as a covering layer to protect lead azide against carbon dioxide (3).

Used in primer blends for non-military ammunition (4).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Voltammetry is now the method of choice for process control, and product control (5). Differential Pulse Polarography, a voltammetric method, is described by Semel (4). No methods for trace analysis were reported.

B. Limit of Detection

Data not available

LEAD STYPHNATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF LEAD STYPHNATE

Chemical	Species	Route	Effects	Reference
Lead styph- ate			No toxicity data located; data on chemical classes and structural analogues follow below	(6)
Lead	Human	inges- tion inhal- ation	General: Pallor, weakness, loss of weight, malnutrition Gastrointestinal: Metallic taste, increased salivation, pyorrhea, anorexia, nausea, vomiting, constipation, abdominal colic and tenderness, Burton's lead line on gums Genitourinary: Nocturia, albuminuria and hematuria, increased bilirubinuria, secondary hyperuricemia, azotemia Neuromuscular: Numbness and tingling of extremities and associated sensory disturbance; extensor weakness of wrists and ankles, brachial palsy has also been described; loss of muscle tone, tremor, increased deep-tendon reflexes, muscular cramps and aching, arthralgia, muscular atrophy Central nervous system: Visual disturbances, headache, dizziness, nervousness or depression, insomnia, mental confusion and delirium, convulsions, coma; encephalopathy may be acute or chronic - acute usually associated with blood levels above 120 ug Pb; retinal hemorrhages and optic neuritis; gray stippling of lead pigment about the optic disc has also been reported	

LEAD STYPHNATE (cont.)

TABLE IV-1. TOXICITY OF LEAD STYPHNATE (Cont.)

Chemical	Species	Route	Effects	Reference
Lead (cont.)	Human	ingestion, inhalation	Hematopoietic: Erythrocyte stippling, hypochromic normocytic anemia, increased peripheral reticulocytes	(7)
Styphnic acid (2,4,6-Trinitroresorcinol)			Unknown (see following table for mutagenicity data)	(8)
Nitrates (As analogue for Styphnic acid)	Human	oral	Large amounts produce dizziness, abdominal cramps, vomiting, bloody diarrhea, weakness, convulsions, and collapse; small repeated doses may lead to weakness, general depression, headache, and mental impairment	(8)
Picric acid (2,4,6-Trinitrophenol) (As analogue for Styphnic acid)	Human	topical	Local or generalized allergic reactions	(9)
	Human	ingestion or percutaneous absorption	Nausea, vomiting, diarrhea, abdominal pain, oliguria, anuria, yellow staining of skin (not icterus), pruritis, skin eruptions, stupor, convulsions, death	(9)
	Various animal species	oral, skin, sc	High acute toxicity	(10) (8)

LEAD STYPHNATE (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF STYPHNIC ACID^a

Test System	Dose	Effects	Reference
<u>Salmonella</u> <u>typhimurium</u> TA98, TA100, TA1535, TA1537 TA1538	NS [*]	Nonmutagenic with or without Aroclor 1254- induced rat liver fraction or treatment with ozone or chlorine	(11)
<u>Salmonella</u> <u>typhimurium</u> TA98, TA100, TA1535, TA1537 TA1538	up to 25 mmol/plate	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(12)
<u>Saccharomyces</u> <u>cerevisiae</u> D3	NS	Did not produce mitotic inhibition with or with- out Aroclor 1254-induced rat liver fraction or treatment with ozone or chlorine	(11)

* No mutagenicity data located on lead styphnate

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

LEAD STYPHNATE (cont.)

B. Effects on animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Concentration of 2,4,6-trinitroresorcinol (styphnic acid) at which inhibition of cell multiplication starts: Bacteria (Pseudomonas putida); 100 mg/L
Algae (Microcystis aeruginosa): 0.32 mg/L (12).
- B7. Aquatic species, fish and invertebrates -- A survey of literature from July, 1974 to the present revealed no data concerning the toxicity of lead styphnate or styphnic acid (trinitroresorcinol) to aquatic organisms (14). The effects of 2,4,6-trinitroresorcinol on fish are LC₅₀, 96 hours; 2.58 mg/L EC₅₀, 96 hours; 0.46 mg/L, behavioral response (12).

C. Effects on Plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Recommended air standard: TWA 0.10 mg(Pb)/m³.

B. Environmental

Reported in EPA TSCA Inventory 1983.

LEAD STYPHNATE (cont.)

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (15).

B. Alternate Disposal Practices Under consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (16).

C. Other Disposal Practices Employed

Destruction of lead styphnate by chemical decomposition: dissolve in at least 40 times its weight of 20% NaOH solution (or in 100 times its weight of 0% ammonium acetate solution) and add sodium dichromate equal to half the weight of lead styphnate, dissolved in 10 parts of tap water (1).

VIII. REFERENCES

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2. Hawley, Gessner G. 1961. The Condensed Chemical Dictionary, 10th ed., p. 609. Van Nostrand-Reinhold, New York, NY.
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LEAD STYPHNATE (cont.)

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16. Forsten, I. 1980. Disposal of Hazardous Toxic Munitions Waste. Proceedings of 1980 National Conference on Enhvironmental Engineering. ASCE Environmental Engineering Division Specialty Conference. 440-575.

LEAD THIOCYANATE

Much of the available data on lead thiocyanate has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{PbC}_2\text{N}_2\text{S}_2$ (1)

Molecular Weight: 323.38 (1)

Structural Formula: $\text{N}\equiv\text{C}-\text{S}-\text{Pb}-\text{S}-\text{C}\equiv\text{N}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 592-87-0

Deleted CAS Registry Number: 10382-36-2

CA Name (9CI): Thiocyanic acid, lead (2+) salt

CA Name (8CI): Same

RTECS Number: Not available on RTECS

Other Significant Synonyms: Lead sulfocyanate (1)

C. Chemical and Physical Properties

Physical State: Powder (1)

Color: White (1)

Odor: Odorless (1)

Melting Point: 190°C decomposes (2)

Solubilities:

Water: In about 200 parts cold; in about 50 parts boiling with decomposition; soluble in alkali hydroxide, nitric acid, and thiocyanate solutions (1).

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: N/A

Hygroscopicity: Data not available

Density (Crystal): 3.82 g/cc (1)

LEAD THIOCYANATE (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Interaction with calcium and magnesium (2). May react with aqueous chlorine to form the highly toxic compound cyanogen chloride (3).

Stability: Data not available

Flammability: Slight, flammable when exposed to heat or flame (2).

II. USES

A. Army Unique Use

Fuel used in detonators, primers and igniters (3).

B. Other Uses

Reverse dyeing with aniline black; manufacture of safety matches and cartridges (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

This compound must be analyzed by determination of the component parts. Lead can be determined by atomic absorption, polarography or colorimetrically as stated in the ARC report (3). For thiocyanate, colorimetric, atomic absorption, and high performance liquid chromatography have been reported. All three methods rely on the formation of a dithiocyanatodipyridyl copper (II) complex, which is detected by each method (4).

B. Limit of Detection

Ingersoll et al. (4) reported 100 ppb.

IV. HEALTH EFFECTS

No data updating the ARC report was found.

LEAD THIOCYANATE (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of lead thiocyanate which would update the Atlantic Research Corporation document. The environmental effects of the compound are chiefly related to the effects of lead, which is highly toxic and bioconcentrative. Toxic combustion products of thiocyanate include cyanide and sulfur oxides.

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 0.15 mg/m³ as lead; STEL 0.45 mg/m³ as lead (5).

B. Environmental

Reported in EPA TSCA Inventory 1983.

Lead thiocyanate has a statutory reportable quantity (RQ) of 5000 lbs under the Comprehensive Environmental Response, Compensation, and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (6).

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (7).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (8).

C. Other Disposal Practices Employed

Convert to nitrates with a minimum of nitric acid (concentrated). Evaporate in a fume hood to a thin paste. Add about 500 mL water and saturate with hydrogen sulfide filter wash and dry the precipitate. Package and ship to the supplier (9).

LEAD THIOCYANATE (cont.)

VIII. REFERENCES

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6. Comprehensive Environmental Response, Compensation and Liability Act, secs. 102 and 103 (1980).
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MAGNESIUM THORIUM ALLOY

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{Mg}_2\cdot\text{Th}$

Molecular Weight: Data not available

Structural Formula: $\text{Mg} \text{---} \text{Th} \text{---} \text{Mg}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 12438-53-8

CA Name (9CI): Magnesium, compound with thorium (2:1); thorium, compound with magnesium (1:2)

CA Name (8CI): Same

RTECS Number: Not available in RTECS

Other Significant Synonyms: None

C. Chemical and Physical Properties

Physical State: Data not available

Color: Data not available

Odor: Data not available

Melting Point: Data not available

Solubilities:

Water: Data not available

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hvgrscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

MAGNESIUM THORIUM ALLOY (cont.)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Casings for electronic weapons systems

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

No analytical methods were found for this compound in a search of the chemical literature from 1967 to the present.

B. Limit of Detection

Data not available

MAGNESIUM THORIUM ALLOY (cont.)

IV. HEALTH EFFECTS

Data on Magnesium thorium alloy was not found. Toxicity of separate parts of the alloy, used as analogues, appears below.

TABLE IV-1. TOXICITY OF MAGNESIUM THORIUM ALLOY

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Magnesium (metal or alloy)	Human	Skin perfor- ation	Partic- ulate form	May produce a severe local lesion charac- terized by the evolution of gas and acute inflam- matory reaction, frequently with necrosis; may cause lymphangitis that is very slow to heal	(1)
Magnesium salts	Human	Intra- venous	Plasma Mg conc. above 2 mmol/L	Symptoms of hypermag- nesemia which may occur include flushing of the skin, thirst, hypotension due to vasodilation, drowsi- ness, loss of tendon reflexes due to neuro- muscular blockade, weakness, respiratory depression, cardiac arrhythmias, coma, and cardiac arrest	(2)
Thorium	Human	NS*	Acute	Has caused dermatitis	(3)
Thorium and thorium compounds	Human	occup. expos- ure	30 yrs; conc. in excess of current standards	No reported toxic effects	(4)
Colloidal thorium dioxide (Thoro- trast)	Human, animal	Injec- tion	NS*	Tumors at various sites attributed to radioactivity	(4) (3)
Thorium compounds	Animal	Various routes	Acute	Low toxicity	(4)

MAGNESIUM THORIUM ALLOY (cont.)

* Not specified

TABLE IV-1. TOXICITY OF MAGNESIUM THORIUM ALLOY (Cont.)

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Thorium compounds (cont.)	Dog	Inhal- ation	26-76 mg/m ³ for 2-10 wk; mean par- ticle dia- meter 1 um	Only toxic effect: abnormal leucocytes	(4)

* Not specified

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of the alloy of magnesium and thorium.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Data not available

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

MAGNESIUM THORIUM ALLOY (cont.)

VIII. REFERENCES

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MIREX

Much of the available data on Mirex has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

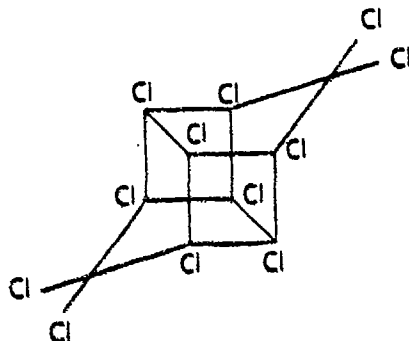
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{10}Cl_{12}$

Molecular Weight: 545.59 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 2385-85-5

Alternate CAS Registry Number: 6842-16-6

Deleted CAS Registry Numbers: 20594-49-4; 56449-78-6; 12557-88-9;
12707-43-6; 12766-04-0

CA Name (9Cl): 1,3,4-Methano-1H-cyclobuta[cd]pentalene,
1,1a,2,2,3,3a,4,5,5,5a,5b,6-dodecachlorooctahydro-

CA Name (8Cl): Same

RTECS Number: PC8225000

Other Significant Synonyms: Dechlorane (1); perchloropentacyclodecane,
perchlorodihomocubane, hexachlorocyclopentadiene dimer

C. Chemical and Physical Properties

Physical State: Crystal (1)

Color: Snow-white (1)

MIREX (cont.)

Odor: Odorless (1)

Melting Point: Decomposes at 485°C (1)

Solubilities:

Water: Practically insoluble

Nonaqueous Solvents: Dioxane 15.3% (room temp.), xylene 14.3% (room temp.), benzene 12.2% (room temp.), carbon tetrachloride 7.2% (room temp.), methyl ethyl ketone 5.6% (room temp.) (1).

Octanol Water Partition Coefficient: LOG P = 6.89 (2)

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: See Section IV, Alb.

Vapor Pressure: 6×10^{-6} mm Hg at 25°C (3)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Reacts with strong oxidizers such as dichromates and chlorine (3).

Stability: Breaks down above 485°C and in sunlight (3).

Flammability: Non-flammable; used as a fire retardant (1).

II. USES

A. Army Unique Use

Fire retardant in tracer ammunitions.

B. Other Uses

Insecticide, fire retardant for plastics, rubber, paint, paper, electrical goods (1).

MIREX (cont.)

III. ANALYTICAL METHODS

A. Acceptable Methods

Gas chromatography (GC) is a well-established technique for analysis of Mirex. Electrolytic conductivity detector is especially well-suited for this poly-chlorinated compound (4). Recent work has resulted in development of a new electrochemical detector for GC that uses a pyrolysis furnace to decompose halogenated compounds with analysis via a potentiometric chloride electrode (5). Driscoll et al. claimed a 1-2 orders of magnitude increase in sensitivity to polychlorinated compounds such as Mirex.

Bush et al. (6) have developed a high performance liquid chromatography method using Ultra Violet (UV) photolysis with electric conductance to measure common pollutants including Mirex at sensitivity of less than 10 nanograms.

Methane chemical ionization (CI) selected ion monitoring (SIM) mass spectrometry is the most sensitive method reported. Hergesheimer reported ppt (parts per trillion) sensitivity for polychlorinated compounds in complex matrices including Mirex (7).

B. Limit of Detection

World Health Organization WHO (4) reported 0.2 pg general and 0.001 micrograms/liter for gas chromatography with electrolytic conductivity detector. Driscoll et al. reported a 1-2 order of magnitude increase over the ECD detector (5).

Bush et al. reported <10 ng for HPLC (6).

Hergesheimer reported parts per trillion for CI-SIM mass spectroscopy (7).

MIREX (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF MIREX*

Species	Route	Dose/Duration	Effects	Reference
Human	oral	50-500 mg/kg	Estimated lethal dose	(8)
NS**	dermal	NS	Moderate skin irritant	(9)
Rat	oral	235-3,000 mg/kg	LD ₅₀	(10)
Rat	oral	50 mg/kg single dose; observed for 28 days	Liver hypertrophy	(11)
Rat (male)	oral (corn oil)	1.0 mg/kg for 14 days	Liver hypertrophy; induction of mixed-function oxidase enzymes	(11)
Rat	oral	5 or 30 ppm in diet for up to 36 mo	No effects on liver weight; proliferation of smooth endoplasmic reticulum after 12 mo	(11)
Rat	oral	50 or 100 ppm in diet for 18 mo; observed until 24 mo	Increased incidence of neoplastic nodules in high-dose male rats; of 17 rats from all groups, 6 animals including 4 high-dose males had liver-cell carcinomas; no metastases were observed	(11)
Rat	NS	Acute	Muscle tremors, diarrhea, and depression followed by death	(11)
Rat (female)	intra-peritoneal	365 mg/kg	LD ₅₀	(11)
Rat	dermal	2,000 mg/kg	LD ₅₀	(11)

* Information not included in the ARC report

** Not specified

MIREX (cont.)

TABLE IV-1. TOXICITY OF MIREX (cont.)

Species	Route	Dose/Duration	Effects	Reference
Mouse	oral	1-90 ppm in diet for up to 70 wk	Increased liver weights at 5 ppm and higher; increased mixed-function oxidase activity, total liver DNA and protein, and mitochondrial respiration at 1 ppm after 70 wk	(12)
Mouse	oral	1-30 ppm in diet for up to 18 mo-	Increased liver weights at 1 ppm in females, at 5 ppm and higher in males; histological changes at 5 ppm and higher; proliferation of smooth endoplasmic reticulum observed ultrastructurally at 1 ppm and above	(12)
Rabbit	dermal	3.33 or 6.7 g mirex bait/kg, 6-7 hr/d, 5 d/wk for 9 wk	No compound-related gross or histopathological changes	(13)
Dog (male)	oral (corn oil)	1,000 mg/kg	LD ₅₀	(13)
Dog	oral	100 ppm in diet for 13 wk	Liver enlargement	(13)
Monkey	oral	0.25 or 1.0 mg/kg, 6d/wk for up to 26 mo	No effect on liver weights, liver histology, or liver ultrastructure	(14)
Hamster	oral	125-250 mg/kg	LD ₅₀	(13)
Duck	oral	2,400 mg/kg	LD ₅₀	(10)
Bird	inhalation	1,400 ppm	LC ₅₀	(10)

* Information not included in the ARC report

** Not specified

MIREX (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF MIREX

Test System	Dose	Effects	Reference
Rat (Wistar) dominant lethal assay	1.5-6 mg/kg/day by gavage for 10 days	Negative	(15)
'Standard Ames bacterial assay"	NS*	Negative; test included liver microsomal activation	(14)

* Not specified

V. ENVIRONMENTAL EFFECTS

This substance has been listed as a carcinogen in the Second Annual Report on Carcinogens (16).

Mirex is covered in the "Preliminary Problem Definition Study on Munitions-Related Chemicals" (1). The ARC report states that Mirex has been used as a pesticide and flame retardant for plastics. The Army's principal current use is in tracer mixes. The material is persistent and mobile in the environment. Its high bioconcentration and biomagnification is noted in the literature. Mirex has been shown to be teratogenic and may also be carcinogenic. Based on the extensive environmental and toxicological studies, use of Mirex has been restricted by the US EPA and the chemical is no longer manufactured in the USA. The small amount used by the military as a tracer is imported.

Mirex is one of the most environmentally stable of the organochlorine insecticides. It degrades slowly and its breakdown products are as toxic and stable as Mirex itself. Mirex bioaccumulates at all trophic levels and biomagnifies in the food chains. Biomagnification in the food chain is enhanced by the delayed mortality typical of Mirex poisoning. Chronic toxicity is a better indicator of the true toxicity of Mirex and is uniformly high (17).

This report is an update; only information since 1978 is discussed below.

A. Environmental Fate

Al. Transport -- Data not available

Als. Adsorption -- Data not available

MIREX (cont.)

- Alb. Volatilization -- Mirex has a very low vapor pressure under normal conditions. The World Health Organization reports that they assume that release of dust is the principal cause of observed airborne Mirex transport (18).
- Alc. Leachability -- Mirex has a very low water solubility. If concentrations exceed 1 ug/l, Mirex would be found in suspended particulate matter. Mirex applied to land has been found to be transported to adjacent water bodies (18).
- Ald. Bioaccumulation -- BCF: algae = 12,200; snails = 4,900; daphnids = 14,650; fish = 2,580; crayfish = 16,860-71,400 (20). as determined with fathead minnow (Pimephales promelas) in 32-day exposures: 18,100 (2).
- A2. Transformation -- Data not available
- A2a. Biodegradation -- Mirex is highly resistant to microbial degradation and thus can persist in soil for long periods. However, it has been reported that in sewage sludge under anaerobic conditions in the dark, about 80% of mirex was degraded into unknown metabolites (19).
- A2b. Hydrolysis -- Aquatic reactions: Exposure to sunlight and UV light have indicated slow degradation; resulting compounds included chlordecone hydrate, undecachloropentacyclodecane, and nonachloropentacyclodecan-5-one hydrate (20).
- A2c. Photolysis -- Mirex undergoes photolytic dechlorination to photomirex (8-monohydroxymirex) and lesser amounts of 5,8-dihydromirex when exposed to sunlight in organic solvent and in duck eggs. Studies examining aged Mirex residues recovered from soil showed fairly large concentrations of photomirex (21).
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- The environmental half-life of Mirex can be many years (22).
- B. Effects on Animals
- B1. Avian species -- Available data indicate low Mirex toxicity to birds (23).
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available

MIREX (cont.)

- B7. Aquatic species fish and invertebrates -- Mirex degradation products were found to be highly toxic for fresh and saltwater bacterial cultures and may be more soluble in water than Mirex itself. Exposure of phytoplankton and algae to Mirex result in reduced productivity and growth rate. Mirex is highly toxic for crustacea. Effects of Mirex on fish are variable (24).

C. Effects on Plants

- C1. Phytotoxicity -- What little work has been done on Mirex effects on terrestrial plants has shown reduction in germination and emergence of grass seeds.
- C2. Uptake -- Available data indicate uptake accumulation and translocation of Mirex in plants (23).
- C3. Metabolism -- Available data indicate no metabolic transformation (23).

VI. STANDARDS AND REGULATIONS

A. Health

Mirex meets criteria for proposed OSHA Medical Records Rule (25) and is included in the Michigan Critical Materials Register.

B. Environmental

Data updating ARC report not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for DDT, a pesticide of related structure, is to dilute or dissolve in a flammable substance, followed by burning in an incinerator equipped with an afterburner and an effluent scrubber. Incineration should be conducted at temperatures exceeding 1000°C with a minimum of 2 seconds dwell time in the combustion zone. Scrubber overflow is to be neutralized prior to discharge. Incinerator ash should be buried in a hazardous or sanitary landfill (26).

While Mirex is known to be resistant to pyrolysis even at temperatures as high as 950°C, it is believed that incineration using the procedure above would destroy most Mirex feed.

B. Alternate Disposal Practices Under Consideration by the Army

Data updating ARC report not available

MIREX (cont.)

C. Other Disposal Practices Employed

Data updating ARC report not available

VIII. REFERENCES

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N-NITROSODIPHENYLAMINE

Much of the available data on N-Nitrosodiphenylamine has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

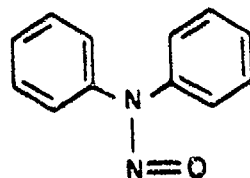
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{12}H_{10}N_2O$

Molecular Weight: 198.22 (estimated)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 86-30-6

CA Name (9CI): Benzenamine, N-nitroso-N-phenyl

CA Name (8CI): Diphenylamine, N-nitroso

RTECS Number: JJ9800000

Other Significant Synonyms: Retarder J, N-Nitroso-N-phenylaniline, Diphenylnitrosamine, N,N-Diphenylnitrosamine, N,N-Diphenyl-N-nitrosamine

C. Chemical and Physical Properties

Physical State: Solid (1)

Color: Yellow to brown or orange powder or flakes (1)

Odor: Mildly amine (1)

Melting Point: 64-66°C (1)

N-NITROSODIPHENYLAMINE (cont.)

Solubilities:

Water: Practically insoluble (1)
Nonaqueous Solvents: Soluble in acetone, benzene, alcohol, and ethylene dichloride. Somewhat soluble in gasoline (1).

Octanol Water Partition Coefficient: $\log P = 3.96$ (2)

Hygroscopicity: Data not available

Density (Crystal): 1.23 g/cc (1)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Comparable to benzene (1)

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

A degradation product of diphenylamine, a propellant (1).

B. Other Uses

Vulcanization retardant in the treatment of rubber. Currently being phased out of industry (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

The Environmental Protection Agency published an official method, number 607, for detection of nitrosamines in water. The method calls for an initial extraction, separation on an alumina column and injection into a gas chromatograph equipped with a nitrogen-phosphorus detector.

N-NITROSODIPHENYLAMINE (cont.)

Difficulty has been reported in separating diphenylamine from N-nitrosodiphenylamine in Method 607 (3). One of the most recent reported methods is a tandem mass spectrometry method by Hunt et al. that eliminated all preparatory steps including chromatography (4).

B. Limit of Detection

EPA Method 607 has been reported to 8.22 ug/l (3). Hunt et al. reported a limit of 10 ppb for their mass spectrometry method (4).

N-NITROSODIPHENYLAMINE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF N-NITROSODIPHENYLAMINE*

Species	Route	Dose/Duration	Effects	Reference
Rat (Fischer 344)	oral	0, 1,000, or 4,000 ppm in feed for 100 wk	Significantly lower survival in high-dose females; significantly increased incidences of transitional-cell car- cinomas of the urinary bladder in high-dose groups; males: con- trols 0/19, low-dose 0/46, high-dose 16/45; females: controls 0/18, low-dose 0/48, high- dose 40/49	(5)
Rat	oral	1,650 mg/kg	LD ₅₀	(6)
Mouse (B ₆ C ₃ F ₁)	oral	Males: 0, 10,000 or 20,000 ppm in feed for 101 wk; Females: 0, 2,315, or 5,741 ppm (time- weighted average) in feed for 98 wk	Chronic inflammatory lesions of the urinary bladder; no significant increases in tumor in- cidences compared with controls	(5)
Mouse	oral	3,850 mg/kg	LD ₅₀	(6)
Rabbit	eye	500 mg/24 hr	Severe irritation	(6)

* Information not included in the ARC report

N-NITROSODIPHENYLAMINE (cont.)

TABLE IV-2. MUTAGENICITY OF N-NITROSODIPHENYLAMINE

Test System	Dose	Effects	Reference
<u>Salmonella typhimurium</u>	50 ug/plate	Mutagenic with microsomes	(6)
Rat embryo cells	1,500 ug/L	Oncogenic transformation	(6)
Rat liver	300 umol/L	DNA Damage	(6)
Rat liver	500 nmol/L	Unscheduled DNA synthesis	(6)
Hamster embryo cells	5,300 ug/L	Oncogenic transformation	(6)
Hamster kidney cells	97 mg/L	Oncogenic transformation	(6)
Hamster fibroblasts	100 umol/L	Sister chromatid exchange	(6)
Various assays in pro-karyotes and eukaryotes for mutagenicity and other chromosomal effects		Negative results	(7)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Log BCF = 2.34, bioconcentration in bluegill sunfish (Lepomis macrochirus), 14-day exposure (8).

A2. Transformation -- Data not available

A2a. Biodegradation -- N-Nitrosodiphenylamine was shown to biodegrade easily. Acclimitization to 5 mg/L in culture media was rapid; acclimitization to 10 mg/L, gradual. Biodegradation in tests ranged from 87% to 100% at 5 mg/L and from 47% to 98% at 10 mg/L dosage (9).

A2b. Hydrolysis -- Data not available

N-NITROSODIPHENYLAMINE (cont.)

- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available
- B. Effects on animals
- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- N-nitrosodiphenylamine was found to be inactive in bacterial DNA repair and reversion tests and yeast mitotic recombination assays made to assess the qualitative nature of the compound's genotoxic potential (10).
- B7. Aquatic species (fish and invertebrates) -- Data not available
- C. Effects on plants
- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

N-Nitrosodiphenylamine has a statutory reportable quantity (RQ) of 1 lb. under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (11).

N-NITROSODIPHENYLAMINE (cont.)

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or, occasionally, hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) which has the responsibility to review current disposal practices and to develop plans for future disposal practices (12).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savannah Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (13).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Kitchens, J.F., W.E. Harwards III, D.M. Lauter, R.S. Valentine. 1978. Preliminary Problem Definition Study of 48 Munitions Related Chemicals, Volume II, Propellant Related Chemicals-N-Nitrosodiphenylamine. Final Report. AD A066308. Atlantic Research Corporation, Alexandria, VA. DAMD17-77-C-7057.
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1-NITRO-2-PROPANOL

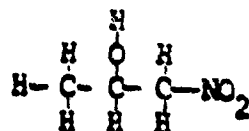
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_3H_7NO_3$

Molecular Weight: 105.09 (Estimated)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 3156-73-8

CA Name (9CI): 2-Propanol, 1-nitro

CA Name (8CI): Same

RTECS Number: Data not available

Other Significant Synonyms: NPL (1)

C. Chemical and Physical Properties

Physical State: Data not available

Color: Data not available

Odor: Data not available

Melting Point: Data not available

Solubilities:

Water: Data not available

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

1-NITRO-2-PROPANOL (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Flash point = 93°C; autoignition temperature = 420°C (1).

II. USES

A. Army Unique Use

Explosive

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

No analytical methods were found in a computerized search of Chemical Abstracts dating back to 1967. Gas chromatography is the most promising technique for development of new methods.

B. Limit of Detection

Data not available

1-NITRO-2-PROPANOL (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF 1-NITRO-2-PROPANOL

Chemical	Species	Route	Effects	Reference
1-Nitro-2-propanol			No toxicity data located; data on analogues appear below.	
Nitrates	Human	oral	Large amounts produce dizziness, abdominal cramps, vomiting, bloody diarrhea, weakness, convulsions, and collapse; small repeated doses may lead to weakness, headache, and mental depression	(2)
2-Nitroethanol	Mouse	intra-peritoneal	LD ₅₀ : 2,000 mg/kg	(3)
2-Nitro-1,3-propanediol	Mouse	intra-peritoneal	LD ₅₀ : 765 mg/kg	(3)
2,2-Dinitro-1-propanol	Mouse	intra-peritoneal	LD ₅₀ : 280 mg/kg	(3)
Isopropyl nitrate	Mouse	inhalation	LC _{Lo} : 65 g/m ³ / 2hr	(3)
<u>n</u> -Propyl nitrate	Rabbit	intra-venous	LD ₅₀ : 200 mg/kg	(3)
	Dog	intra-venous	LD _{Lo} : 200 mg/kg	(4)
	Cat	intra-venous	LD _{Lo} : 100 mg/kg	(4)

1-NITRO-2-PROPANOL (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of 1-nitro-2-propanol.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or, occasionally, hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (5).

B. Alternate Disposal Practices Under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (6).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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1-NITRO-2-PROPANOL (cont.)

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2-NITRODIPHENYLAMINE

Much of the available data on nitrodiphenylamine has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

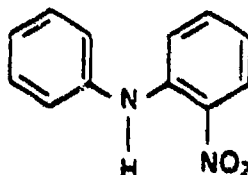
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{12}H_{10}N_2O_2$

Molecular Weight: 214.24

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 119-75-5

CA Name (9CI): Benzenamine, 2-nitro-N-phenyl

CA Name (8CI): Diphenylamine, 2-nitro

RTECS Number: Not available on RTECS

Other Significant Synonyms: o-Nitro-N-phenylaniline, o-Nitrodiphenylamine, 2-Nitro-N-phenyl benzenamine

C. Chemical and Physical Properties

Physical State: Crystalline powder (1)

Color: Red-brown (1)

2-NITRODIPHENYLAMINE (cont.)

Odor: Data not available

Boiling Point: 224°C (2)

Melting Point: 75-76°C (1)

Solubilities:

Water: Data not available

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Log P = 4.60 (estimated)

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Reactivity: Combustible

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Slight (2)

II. USES

A. Army Unique Use

Data not available

B. Other Uses

Stabilizer for nitroglycerin, chemical intermediate.

2-NITRODIPHENYLAMINE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Bender reported qualitative and quantitative determinations of 2-nitrodiphenylamine and other components of smokeless powders by high performance liquid chromatography with ultraviolet or thermal energy analyzer detectors.

Thin-layer chromatography and high performance thin-layer chromatography with liquid chromatography, have been reported by Ammann et al. to analyze the stabilizers in double-base propellants including 2-nitrodiphenylamine.

B. Limit of Detection

Reductive and oxidative electrochemical detection with liquid chromatography is applied to the determination of explosives-e.g. nitroglycerin, 2,4-dinitrotoluene and diphenylamine in military explosives and single- and double-base smokeless gunpowders (3).

2-NITRODIPHENYLAMINE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. MUTAGENICITY AND RELATED EFFECTS OF 2-NITRODIPHENYLAMINE*

Test System	Dose	Effects	Reference
<u>E. coli</u> W3110/poIA ⁺ p3478/poIA	100 ug- 10 mg	Not active with or without Aroclor 1254-induced rat liver S9	(4)
<u>S. typhimurium</u> TA100, TA1535, TA1537, TA1538	NS**	Nonmutagenic with or without Aroclor 1254-induced rat liver S9	(4)
<u>S. cerevisiae</u> D5	NS	Did not produce mitotic recombination with or without Aroclor 1254-induced rat liver S9	(4)

* Information not included in the ARC report

** Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

2-NITRODIPHENYLAMINE (cont.)

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- 2-Nitrodiphenylamine was found to be inactive in bacterial DNA repair and reversion tests and yeast mitotic recombination assays made to assess the qualitative nature of the compound's genotoxic potential (4).
- B7. Aquatic species fish and invertebrates -- Data not available
- C. Effects on plants
 - C1. Phytotoxicity -- Data not available
 - C2. Uptake -- Data not available
 - C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (5).

2-NITRODIPHENYLAMINE (cont.)

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (6).

C. Other Disposal Practices Employed

For 4-nitrodiphenylamine, the following disposal method is given: Dissolve or mix the material with a combustible solvent and burn in an incinerator equipped with an afterburner and scrubber (7). Also, Eastman Kodak Company recommends disposal in an approved incinerator equipped with an afterburner and a scrubber (8).

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8. KODAK Laboratory Chemicals Catalog No. 52. 1985. Chemical No. 3906, p. 372. Eastman Kodak Company, Rochester, NY.

OCTACHLOR CARBANILIDE

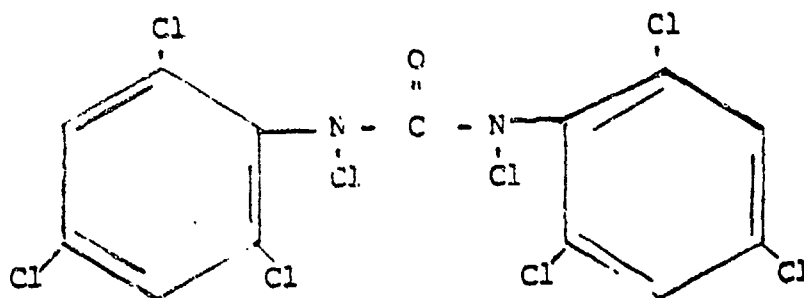
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{13}H_4Cl_8N_2O$

Molecular Weight: 487.8 (estimated)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 2899-02-7

Ca Name (9CI): Urea, N,N'-dichloro-N,N'-bis (2,4,6-trichlorophenyl)-

CA Name (8CI): Carbanilide, (N,N',2,2',4,4',6,6'-) octachlor

RTECS Number: Not in RTECS

Other Significant Synonyms: CC2, Sym-dichlorobis (2,4,6-trichlorophenyl) urea

C. Chemical and Physical Properties

Physical State: Solid (1)

Color: White, turns pink to red with decomposition (1)

Odor: Chlorine (1)

Melting Point: Decomposes on heating above 150°C (1)

OCTACHLOR CARBANILIDE (cont.)

Solubilities:

Water: Insoluble (1)

Nonaqueous Solvents: Not ethanol; glacial acetic acid (1)

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Not hygroscopic

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: 2mm Hg (1)

Specific Heat: 43 kcal/mole (1)

Heat of Combustion: Data not available

Reactivity: Explosive with compounds that react with chlorine (1).

Octachlor carbanilide reacts explosively with dimethylsulfoxide (DMSO) (2).

Stability: Unstable; decomposes photochemically and in the presence of oxygen. Must be kept in dark and under vacuum (1).

Flammability: Data not available

II. USES

A. Army Unique Use

Chlorinating Agent (1); ingredient in anti-chemical agent impregnation mixture, often used to impregnate clothing.

B. Other Uses

Potential use as fire retardant, bactericide, and anti-vesicant (3).

III. ANALYTICAL METHODS

A. Best Acceptable Method

No methods of analysis were found in a search of Chemical Abstracts from 1967 through the present.

B. Limit of Detection

Data not available

OCTACHLOR CARBANILIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF OCTACHLOR CARBANILIDE

Chemical	Species	Route	Effects	Reference
Octachlor carbanilide (<u>N,N'</u> ,2,2',4,4',6,6'- Octachlorocarbanilide)			No toxicity data located; data on structural analogues and chemical classes follow below	
2,2',4,4',6,6'-Hexachlorocarbanilide	Rat	oral	Mortality: 1/10 at 50 mg/kg, 0/10 at 100 mg/kg	(4)
2,3',4'-Trichlorocarbanilide	Mouse	intravenous	LD ₅₀ : 63 mg/kg	(4)
3,4,4'-Trichlorocarbanilide	Mouse	intraperitoneal	LD ₅₀ : 2,100 mg/kg	(4)
1,2,3-Trichlorobenzene, 1,3,5-Trichlorobenzene	NS*	NS	Moderate irritant to skin, eyes, and mucous membranes; causes hair loss; liver injury has been reported with 1,2,3-trichlorobenzene	(5)
Hypochlorous acid (available chlorine)	Human	local	Highly irritating to skin, eyes, and mucous membranes	(6)
	Human	ingestion	Irritation and corrosion of mucous membranes with pain and vomiting; a fall in blood pressure, delirium, and coma may occur	(7)
	Human	inhalation	Coughing, choking; may cause severe respiratory tract irritation and pulmonary edema	(7)

OCTACHLOR CARBANILIDE (cont.)

V. ENVIRONMENTAL EFFECTS

Little information was found regarding the environmental fate or effects of octachlor carbanilide.

Octachlor carbanilide decomposes at high temperature with the formation of Sym-2,4,6-trichlorophenyl urea (8).

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

The disposal practice recommended by the U.S. Navy in their Consolidated Hazardous Item List for Impregnite, a related compound used for a similar purpose, is burning in an incinerator equipped with an effluent scrubber. Scrubber overflow is to be neutralized prior to discharge. Incinerator ash should be buried in a hazardous or sanitary landfill (9).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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OCTACHLOR CARBANILIDE (cont.)

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p-NITROPHENOL

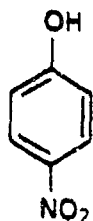
I. . CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_5NO_3$ (1)

Molecular Weight: 139.11 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 100-02-7

CA Name (9CI): Phenol, 4-nitro

CA Name (8CI): Phenol, p-nitro

RTECS Number: SM2275000

Other Significant Synonyms: p-Hydroxynitrobenzene; 4-hydroxynitrobenzene

C. Chemical and Physical Properties

Physical State: Crystals (1)

Color: Colorless to slightly yellow (1)

Odor: Odorless (1)

Melting Point: 113-114°C; sublimes (1)

p-NITROPHENOL (cont.)

Boiling Point: 279°C; decomposes (2)

Solubilities:

Water: Slightly soluble in cold water; soluble in solutions of fixed alkali hydroxide and carbonates (1): 1.6% at 25°C; 2.7% at 90°C (3).

Nonaqueous Solvents: Soluble in alcohol, chloroform, ether (1).

Octanol Water Partition Coefficient: Log P = 1.91 (4)

Dissociation Constant: 7.0×10^{-8} (5)

Hygroscopicity: Data not available

Density (Crystal): 1.270 g/cc

Volatility: Sublimes (1)

Vapor Pressure: Less than 1 mm Hg at 38°C

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Slightly flammable; combustible solid, may thermally decompose in absence of air (3).

II. USES

A. Army Unique Use

Explosive

B. Other Uses

Acid-base indicator (0.1% alcohol solution, pH: 5.6, colorless; pH: 7.6, yellow) (1). Intermediate in organic synthesis; production of parathion; fungicide for leather (3).

p-NITROPHENOL (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Two high pressure liquid chromatographic methods for determining p-nitrophenol in complex wastewater matrices have been reported. Nielsen et al. (6) reported that using precolumn separation and diode-array detection, 29 chemicals found in wastewater, including p-nitrophenol, can be separated and quantitized in a fully automated system. Kruempelman and Danielson (7) reported the use of Picolyl Kel-f to separate nitrophenols.

Eichelberger et al. (8) reported success using both packed column and fused silica capillary column GC/MS. Chudyk et al. (8) reported detecting p-nitrophenol in contaminated groundwater in situ at a depth of 25 m by laser-induced fluorescence at below parts-per-billion level.

B. Limit of Detection

Eichelberger et al. (8) reported 16.3 micrograms/liter for the packed column method and 20 micrograms/liter for the capillary column.

p-NITROPHENOL (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF P-NITROPHENOL

Species	Route	Effects	Reference
Human	inhalation, ingestion, skin	Headache, drowsiness, nausea, loss of consciousness; blue color in lips, ears, and fingernails (cyanosis)	(10)
Human	local	Dust is irritating to eyes, nose, and throat; solid is irritating to skin and eyes	(10)
Human	oral	Estimated lethal dose: 50-500 mg/kg	(10)
Test animals	NS*	Central and peripheral vagus stimulation, central nervous system depression, methemoglo- binemia, dyspnea, and hyper- thermia	(12,13)
Rat	oral	LD ₅₀ : 350 mg/kg	(14)
Rat	subcutaneous	LD _{Lo} : 200 mg/kg	(14)
Mouse	oral	LD ₅₀ : 380 mg/kg	(14)
Mouse	intra- peritoneal	LD ₅₀ : 75 mg/kg	(14)
Guinea pig	subcutaneous	LD _{Lo} : 200 mg/kg	(14)
Dog	intravenous	LD _{Lo} : 10 mg/kg	(14)
Cat	NS	LD ₅₀ : 150 mg/kg	(14)
Pigeon	intra- muscular	LD _{Lo} : 65 mg/kg	(14)
Frog	subcutaneous	LD _{Lo} : 60 mg/kg	(14)

* Not specified

p-NITROPHENOL (cont.)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF p-NITROPHENOL

Test System	Dose	Effects	Reference
<u>Escherichia coli</u>	50 umol/L	Induction of DNA damage	(14)
Microorganism (unspecified)	10 mg/plate	Effects on DNA repair	(14)
Hamster fibroblasts	1 mmol/L	Inhibition of DNA synthesis	(14)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

Al. Transport

Ala. Adsorption -- Tests performed on four soil types reported that p-nitrophenol appears to follow a Freundlich Isotherm for soil adsorption. Freundlich parameters k and n appear to correlate with Hammet (G) and hydrophobic (pi) parameters (5).

Alb. Volatilization -- Data not available

Alc. Leachability -- Data not available

Ald. Bioaccumulation -- The strongly hydrophobic nature of p-nitrophenol suggests that it could accumulate in cell lipids, particularly membrane lipid bilayers. The kinetics of killing of cultured mammalian cells revealed that the cells became more sensitized to the pollutant with time of exposure, and this may also reflect a time-dependent accumulation of the compound into the hydrophobic regions of the membranes (15).

A2. Transformation -- Data not available

A2a. Biodegradation -- Adapted culture: 2% removal after 48-hour incubation, feed: 200 mg/L. Decomposition by a soil microflora in 16 days. Adapted activated sludge at 20°C, with p-nitrophenol as sole carbon source: 95.0% COD removal at 17.5 mg COD/g dry inoculum/hr. Lag period for degradation of 16 mg/L by wastewater at pH 7.3, 30°C: 3-5 days; soil suspension at pH 7.3, 30°C: 7-14 days. P-Nitrophenol was found to biodegrade rapidly under both aerobic and anaerobic conditions in the presence of exogenous organic nutrients, but its persistence increased considerably in the absence of such nutrients (17).

p-NITROPHENOL (cont.)

- A2b. Hydrolysis -- Data not available
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available

B. Effects on Animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- The o-, m- and p-nitrophenols reduce the rate of algal photosynthetic oxygen production by as much as 70% at the relatively high exposure of 50-100 mg/L (18).

Toxicity threshold (cell multiplication inhibition test): bacteria (Pseudomonas putida), 4 mg/L; algae (Microcystis aeruginosa), 56.0 mg/L; green algae (Scenedesmus quadricauda), 7.4 mg/L; protozoa (Entosiphon sulcatum), 0.83 mg/L; protozoa (Uronema parduczi Chatton-Lwoff), 0.89 mg/L (16).

- B7. Aquatic species, fish and invertebrates -- Fish: Vairon (F): TLM 6 hr: distilled water: 4-6 mg/L; hard water: 30-33 mg/L (16).

Daphnia magna: 24-hour LC_{50} : 24000 ug/L (19).

Lepomis macrochirus: 24-hour LC_{50} : 12000 ug/L; 96-hour LC_{50} : 8300 ug/L (21).

Shrimp (Cragdon septemspinosa): 96-hour Lethal threshold: 26.4 mg/L;
Clam (Mya arenaria): 96-hour Lethal threshold: 29.4 mg/L; (22)

C. Effects on Plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

p-NITROPHENOL (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

The compound p-nitrophenol has a statutory reportable quantity (RQ) of 1 lb. under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (23).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (24).

B. Alternate Disposal Practices Under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (25).

C. Other Disposal Practices Employed

Wastewater treatment: ion exchange; adsorption on Amberlite XAD-2; 100% retention effective; influent 0.2ppm, effluent nil (19).

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p-NITROPHENOL (cont.)

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PENTAERYTHRITOL TETRANITRATE

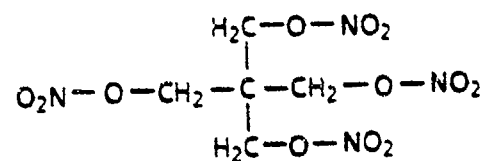
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_5H_8N_4O_{12}$

Molecular Weight: 316.17

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 78-11-5

CA Name (9CI): 1,3-propanediol, 2,2-bis (nitrooxy) methyl-dinitrate (ester)

CA Name (8CI): Pentaerythritol, tetranitrate

RTECS Number: RZ2623000

Other Significant Synonyms: 2,2-Bis(dihydroxymethyl)-1,3-propanediol, tetranitrate; Nitropentaerythritol; PETN

C. Chemical and Physical Properties

Physical State: Tetragonal crystals (1)

Color: White (2)

Odor: Odorless

Melting Point: $141^{\circ}C$ (2)

PENTAERYTHRITOL TETRANITRATE (cont.)

Solubilities:

Water: Practically insoluble (3); 0.01g/100 g at 50°C
Nonaqueous Solvents (20°C): Acetone, 24.95% (very soluble); methyl acetate, 13%; beta-ethoxy ethyl acetate, 1.5% (2)

Octanol Water Partition Coefficient: $\log P = 0.59$ (4)

Hygroscopicity: 0 at 30°C, 90% relative humidity (2)

Density (Crystal): 1.77 g/cc (2)

Volatility: Nonvolatile (2)

Vapor Pressure (p): Below measurable limits.

Specific Heat: 0.26 cal/g/°C (2)

Heat of Combustion: 1,960 cal/g (2)

Reactivity: The explosion hazard is severe when shocked or exposed to heat. One of the most powerful high explosives, it is particularly sensitive to shock. Explodes at 205-215°C. On decomposition, emits highly toxic fumes of NO_x ; can react vigorously with oxidizing materials (5).

Stability: Due to its symmetrical structure, PETN is highly resistant to many reagents. PETN differs from the majority of nitrate esters because it is not readily decomposed by sodium sulfide at 50°C. It is decomposed quickly, however, by boiling in a ferrous chloride solution. Boiling with a 2.5% solution of sodium hydroxide causes very slow decomposition.

PETN is hydrolyzed by treatment with water at approximately 100°C. At 125°C under pressure, hydrolysis proceeds quickly and is considerably enhanced by the presence of 0.1% HNO_3 . A dilute sodium hydroxide solution causes PETN to hydrolyze more rapidly than acidified water. Hydrolysis produces mainly pentaerythritol dinitrate (6).

Flammability: Will not continue to burn (2)

II. USES

A. Army Unique Use

PETN is used in Class A-detonating fuse and boosters and Class B-priming compositions, as a bases charge in anti-aircraft shells and mixed with TNT (70-30) in mines, explosive bombs and torpedoes. It is a very effective demolition explosive. It is also used in blasting caps combined with lead azide and diazodinitrophenol. PETN was known as an explosive in 1894; it was not used on a practical basis until after World War I (5,2).

PENTAERYTHRITOL TETRANITRATE (cont.)

B. Other uses

PETN is used therapeutically in the treatment of angina pectoris (7).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Several chromatographic methods were reported in recent literature. Lloyd reported an high performance liquid chromatography method that uses a pendant mercury drop electrode at the detector. This method compared favorably with electron capture detection in gas chromatography (8).

A Thermal Energy Analyzer (TEA) interfaced with a gas or liquid chromatograph was reported by Fine et al. (9) to detect explosives in debris without prior clean-up.

Yu et al. (10) reported a method to determine this compound with nitro/nitroso specific detector with either a gas or liquid chromatograph. This method can be used in the analysis of wastewater or biological fluids. The detector is a TEA and can also be applied to metabolites of nitrate esters.

Cantu et al. (11) reported success using a Fourier transform infrared spectrometer coupled with HPLC.

Yinon (12) described a custom built mass spectrometer interfaced with an HPLC that can successfully analyze PETN and other explosives. Cumming and Park (13) reported a gas chromatography/single ion monitoring mass spectroscopy method.

Malotky and Downes (14) reported a field kit for the analysis of 28 different explosives, including PETN, using thin-layer chromatography.

B. Limit of Detection

Lloyd (8) reported a detection limit of 2-20 picogram/10 microliters of injected sample.

Fine et al. (9) reported a detection limit of <10 picograms.

PENTAERYTHRITOL TETRANITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF PENTAERYTHRITOL TETRANITRATE

Species	Route	Dose/Duration	Effects	Reference
Human	oral	Therapeutic dose levels	Cutaneous vasodilation; rash; headache; increased intraocular pressure; dizziness, weakness, other signs of cerebral ischemia associated with postural hypotension	(7, 15)
Human (63-yr-old man)	oral	10 mg, 4x/d, x8 yr; with glyceryl trinitrate, 1 or 2x/mo	Erythroderma	(16)
Human (74-yr-old man)	oral	80 mg/d	Rosacea with strong flushing	(17)

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF PENTAERYTHRITOL TETRANITRATE

Test System	Dose	Effects	Reference
<u>Salmonella typhimurium</u> TA98, TA100, TA1535, TA1537, TA1538	NS*	Nonmutagenic with or without Aroclor 1254-induced rat liver fraction or treatment with ozone or chlorine	(18)
<u>Salmonella typhimurium</u> TA98, TA100, TA1535, TA1537, TA1538	0.625, 1.25 mg (spot test); up to 2.5 mg/plate (plate incorporation assay)	Nonmutagenic with or without Aroclor 1254-induced rat liver S9	(19)
<u>Saccharomyces cerevisiae</u> D3	NS	Did not produce mitotic inhibition with or without Aroclor 1254-induced rat liver fraction or treatment with ozone or chlorine	(18)

* Not specified

PENTAERYTHRITOL TETRANITRATE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Non-volatile (2)

A1c. Leachability -- Insoluble in water (6)

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Studies in rats have shown that PETN is degraded to the mono-, di-, and tri-nitrates by the bacterial flora of the intestine. Studies both in vivo and in vitro have indicated that nitrite rather than nitrate is the product of biodegradation of PETN (20).

A2b. Hydrolysis -- The water solubility of PETN is so low (about 2 mg/L at 20°C), that almost all hydrolysis studies have been carried out in mixed solvents at reflux temperatures, and reactions were promoted by strong acid or base. Therefore, the experimental data are not directly applicable to the assessment of hydrolysis of PETN in natural waters and wastewaters (20).

A2c. Photolysis -- Burrows and Dacre report that there have been studies of the decomposition of solid PETN exposed to ultraviolet light, but they state that it is not known whether this relates in any way to degradation of dissolved PETN or its metabolites in the environment (20).

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

PENTAERYTHRITOL TETRANITRATE (cont.)

- B7. Aquatic species, fish and invertebrates -- Water flea (Daphnia magna): 48-hour LC₅₀: 292 mg/L; Bluegill (Lepomis macrochirus): 96-hour LC₅₀: >2230<3430⁵⁰ mg/L; Fathead minnow (Pimephales promelas): 96-hour LC₅₀: 926 mg/L (21).

C. Effects on plants

- C1. Phytotoxicity -- Data not available
C2. Uptake -- Data not available
C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (22).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (23).

C. Other Disposal Practices Employed

Data not available

PENTAERYTHRITOL TETRANITRATE (cont.)

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PENTAERYTHRITOL TETRANITRATE (cont.)

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PHOSPHORUS TRICHLORIDE

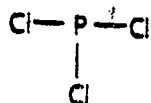
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: PCl_3

Molecular Weight: 137.35 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 7719-12-2

Deleted CAS Registry Number: 11082-95-4

CA Name (9CI): Phosphorus trichloride

CA Name (8CI): Phosphorus chloride

RTECS Number: TH3675000

Other Significant Synonyms: Phosphine, trichloro-, phosphorus chloride

C. Chemical and Physical Properties

Physical State: A fuming liquid (1)

Color: Colorless (1)

Odor: Data not available

Melting Point: -112°C (1)

Boiling Point: 76°C (1)

Solubilities:

Water: Decomposes (1)

Nonaqueous Solvents: Decomposes in alcohol (1); soluble in benzene, ether, chloroform, carbon disulfide (1); soluble in carbon tetrachloride (2)

PHOSPHORUS TRICHLORIDE (cont.)

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Decomposes on contact with water (1)

Specific Gravity: 1.574 (1)

Volatility: Fuming (1)

Vapor Pressure: 100 mm at 21°C (1); 400 mm at 56.9°C (3); vapor density 4.75 g/L (3)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Nonflammable (3)

II. USES

A. Army Unique Use

Obscurants and chemical intermediates.

B. Other Uses

Same uses as phosphorus oxychloride (chlorinating agent); in the manufacture of phosphorus pentachloride and phosphorus oxychloride, producing iridescent metallic deposits (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Phosphorus can be detected in trace amounts by atomic emission spectrometry. Hee et al. recently reported a simultaneous inductively coupled plasma atomic emission spectrometric method for phosphorus and 33 other elements (4).

B. Limit of Detection

Hee et al. reported a lowest quantifiable limit (LQL) of less than 0.1 microgram per milliliter (4).

PHOSPHORUS TRICHLORIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF PHOSPHORUS TRICHLORIDE

Species Reference	Route	Dose/Duration	Effects	
Human	contact with vapor	NS*	Highly irritating to skin, eyes, throat, and respiratory tract	(5)
Human	contact with liquid	NS	Severe burns of the eyes and skin	(5)
Human	inhalation	Minor exposures	Acute pulmonary edema; may be delayed 2-6 hr	(6)
		Moderate to severe exposures	Acute pulmonary edema; may be delayed 12-24 hr	(6)
Human (27 patients)	inhalation	Exposure following a railroad yard accident	Effects included burning eyes, shortness of breath, throat irritation, eye lacrimation, headache, nausea, burning skin, sputum production, generalized chest pain, pleuritic chest pain, rash with or without itch, wheezing, blurred vision, vomiting, abdominal pain, pulmonary changes, hypoxemia	(7)
Human (chemical workers)	inhalation	Intermittent exposure to PCl_3 and $POCl_3$ concentrations of PCl_3 exceeded 3 mg/ m^3 standard in 2 of 13 air samples in original study (respirators worn in these cases); no air sampling in follow-up study	Increased incidences of respiratory distress consisting of wheezing, breathlessness, and chest tightness in 37 exposed vs. 22 unexposed workers in original study and in 26 exposed vs. 11 unexposed workers 2 years later in a follow-up study	(8)

* Not specified

PHOSPHORUS TRICHLORIDE (cont.)

TABLE IV-1. TOXICITY OF PHOSPHORUS TRICHLORIDE (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Rat	oral	550 mg/kg	LD ₅₀	(9)
Rat	inhalation	104 ppm/4 hr	LC ₅₀	(9)
Guinea pig	inhalation	50 ppm/4 hr	LC ₅₀	(9)

* Not specified

TABLE IV-2. MUTAGENICITY OF PHOSPHORUS TRICHLORIDE

Test System	Dose	Effects	Reference
<u>Salmonella</u> <u>Oyphimurium</u> (8 strains); <u>Escherichia</u> <u>coli</u> (2 strains)	0.1-1,000 ug/ml; gradient plate method	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(10)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Decomposes in water to hydrochloric acid and H₃PO₄ (3).

A2c. Photolysis -- Data not available

PHOSPHORUS TRICHLORIDE (cont.)

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Data not available

B6. Microorganisms, aquatic and soil -- Data not available

B7. Aquatic species, fish and invertebrates -- Data not available

C. Effects on plants

C1. Phytotoxicity -- Data not available

C2. Uptake -- Data not available

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Phosphorus trichloride has a statutory reportable quantity (RQ) of 5000 lb under the Comprehensive Response, Compensation and Liability Act. The National Response Center must be notified when there is a release of this compound in an amount equal to or greater than the RQ (11).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

A recent programmatic life cycle environmental assessment indicates that incineration is the preferred method for disposal of smoke/obscurant munitions. Munitions containing phosphorus would be incinerated in a unit equipped with afterburner and a scrubber (12).

PHOSPHORUS TRICHLORIDE (cont.)

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Phosphorus trichloride can be syphoned into a running stream and neutralized. However, the danger of forming explosive or toxic fumes dictates the work be done in an isolated area with all personnel adequately protected (3). (Editor's note: The recommendation that the material be neutralized is very important when using this disposal method; the pre-disposal pH of the stream should be maintained. This method may contribute to algal growth downstream due to excessive phosphorus application.)

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PHOSPHORUS TRICHLORIDE (cont.)

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POTASSIUM DINITROBENZFUROXAN

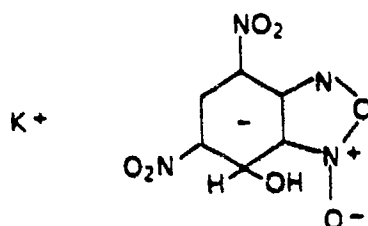
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_4N_4O_6K$ (1), $C_6H_3N_4O_7K$ (2)

Molecular Weight: 225 (1), 282 (Estimated)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 29267-75-2

CA Name (9CI): 4-Benzofurazan-ol, 1-4-dihydro-5,7-dinitro, 3-oxide, ion(-1) potassium

CA Name (8CI): Benzofurazan, 4,6-dinitro-1-oxide, potassium salt*

RTECS Number: Not applicable

Other Significant Synonyms: KDNEF

C. Chemical and Physical Properties

Physical State: Crystalline solid (1)

Color: Golden orange (1)

Odor: Data not available

Melting Point: 230°C (Explodes) (1)

POTASSIUM DINITROBENZFUROXAN (cont.)

Solubilities:

Water: 0.245 g/100 g at 30°C (1)

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: At 30°C -- 75% Relative humidity -- 0.11%

90% Relative humidity -- 0.27% (1)

Density (Crystal): 2.21 g/cc (1)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: 0.217 cal/g/°C (1)

Heat of Combustion: 2209 cal/g (1)

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Primary explosive (1)

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

None found under name or CAS registry number.

B. Limit of Detection

None found under name or CAS registry number.

POTASSIUM DINITROBENZFUROXAN (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF POTASSIUM DINITROBENZFUROXAN

Chemical	Effects	References
Potassium dinitro-hydroxy hydro-benzofuroxan	Moderately toxic by inhalation and ingestion	(3)
4,6-Dinitrobenzo-furoxan	Inhibition of RNA synthesis in sheep lymphocytes <u>in vitro</u> : 5% inhibition at 20 uM, 95% inhibition at 100 uM; reacts with nucleophiles	(4)
4-Nitrobenzofuroxan	Mutagenic in <u>Salmonella typhimurium</u> strains TA98, TA100, TA1530R, TA1535R ⁺	(5)
	Inhibition of DNA synthesis in mouse leukocytes	(6)
4-Nitrobenzofuroxan	Inhibition of nucleic acid and protein synthesis in animal cells	(4)
Nitrates	Large amounts taken by mouth produce dizziness, abdominal cramps, vomiting, bloody diarrhea, weakness, convulsions, and collapse; small, repeated doses may lead to weakness, general depression, headache, and mental impairment	(7)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of potassium dinitrobenzofuroxan.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (8).

B. Alternate Disposal Practices Under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (9).

C. Other Disposal Practices Employed

Data not available

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POTASSIUM PERCHLORATE

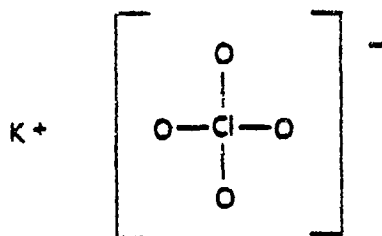
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: KClO_4

Molecular Weight: 138.55

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 7778-74-7

CA Name (9CI): Perchloric acid, potassium salt

CA Name (8CI): Perchloric acid, potassium salt

TECS Number: SC9700000

Other Significant Synonyms: Potassium hyperchloride; Potassium hyperchlorate.

C. Chemical and Physical Properties

Physical State: Rhombic crystals or white crystalline powder (1)

Color: Colorless or white

Odor: Odorless (2)

Melting Point: $610-620^\circ\text{C}$ (3)

Boiling Point: Data not available

Solubilities:

Water: Soluble in 65 parts cold and in 15 parts boiling water (1)

Nonaqueous Solvents: Very slightly soluble in alcohol and insoluble in ether (4). Insoluble in alcohol (1).

POTASSIUM PERCHLORATE (cont.)

Density: 2.52 g/cc (5)

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Decomposed by organic matter and agents subject to oxidation; strong oxidizing agent (5); violent reaction with aluminum and magnesium, fluorine, nickel and titanium (3).

Stability: Decomposed by concussion (1); decomposes at 400 °C (4); decomposes at 530 °C (6); moderate explosion hazard (6).

Flammability: Data not available

II. USES

A. Army Unique Use

Pyrotechnics, oxidizer for rocket propellant

B. Other Uses

Fireworks, pharmaceuticals, oxidizing agent, analytical reagent.

III. ANALYTICAL METHODS

There is an ion chromatography method for determining potassium perchlorate in Pyrodex, a commercial black powder substitute. This method was developed for trace forensic analysis of black powders and their combustion products and residues.

B. Limit of Detection

Data not available

POTASSIUM PERCHLORATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF POTASSIUM PERCHLORATE

Species	Route	Dose/Duration	Effects	Reference
Human	oral	Therapeutic	Nausea, vomiting, and hypersensitivity reactions such as maculopapular rashes, fever, and lymphadenopathies may occur; fatal aplastic anemia has occurred in a small proportion of patients; agranulocytosis, thrombocytopenia, and leucopenia have been reported.	(2)
72-yr-old female (treated for thyrotoxicosis)		1g/d for 1 month then 200 mg/d for 22 yr	No toxic effects	(7)
Human	inhalation with dust, oral	NS*	Irritation of skin, contact eyes, and mucous membranes; absorption can produce methemoglobinemia and kidney injury	(3)
Rat	oral	27,675 mg/kg gestation days 1-9	TD _{Lo} for developmental abnormalities	(8)
Rat	intra-peritoneal	10 mg	Antithyroid activity	(9)
Rabbit	oral	2,100 mg/kg, gestation days 1-21	TD _{Lo} for developmental abnormalities	(8)
Guinea pig	oral	35,700 mg/kg, gestation days 48-68	TD _{Lo} for developmental abnormalities	(8)

POTASSIUM PERCHLORATE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- A few microorganisms are able to metabolise perchlorate; most are not. It has been reported that perchlorate is reduced to chloride by several species of heterotrophic bacteria, including the very common E. coli and Pseudomonas aeruginosa. Some Streptococcus and Flavobacterium spp. were inactive (10).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

B5. Amphibians -- Newts maintained at a level of 36 mg/L of perchlorate exhibit significant histological changes in the thyroid and pituitary. Continuous exposure to 360 mg/L results in arrested metamorphosis in tadpoles and a grossly enlarged thyroid in guppies (10).

B6. Microorganisms, aquatic and soil -- Toxicity thresholds, by cell multiplication inhibition test: bacteria (Pseudomonas putida): 1870 mg/L; green algae (Scenedesmus quadricauda): 360 mg/L; protozoa (Entosiphon sulcatum): 23 mg/L (11).

POTASSIUM PERCHLORATE (cont.)

- B7. Aquatic species (fish and invertebrates) -- LC₅₀ for Daphnia magna in 24-hour exposure = 670000 ug/L (calc.) (12).

Although few definitive studies have been conducted, it appears that the acute toxicity of perchlorate ion to aquatic animals and microorganisms is very low, with toxic levels probably exceeding 1000 mg/L for periods of 24 hours and longer. Because perchlorate is an important antithyroid agent, chronic effects may appear at much lower levels. Guppies (Lebistes reticulatus) exposed to 500 mg/L of potassium perchlorate for a year and longer suffered gross enlargement of the thyroid, followed by inactivation of the thyroid and arrested sexual development (10).

C. Effects on plants

- C1. Phytotoxicity -- Soybeans grown in water culture exhibit toxic symptoms at perchlorate levels as low as 2.5 mg/L four days after application. Soybeans grown in sand were noticeably less susceptible (10).
- C2. Uptake -- Uptake of iodide by the seaweed Fucus ceranoides is competitively inhibited by perchlorate at the 0.1 mg/L level in seawater (10).
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Current methods of disposal of pyrotechnics involves open burning or open detonation.

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

POTASSIUM PERCHLORATE (cont.)

C. Other Disposal Practices Employed

Use vast volume of concentrated solution of reducing agent (bisulfites or ferrous salts with 3M-H₂SO₄ or hypc). Neutralize with soda ash or dilute HCl. Drain into a sewer with abundant water (13).

For small quantities: Cautiously add to a large stirred excess of water. Adjust the pH to neutral, separate any insoluble solids or liquids and package them for hazardous waste disposal. Flush the aqueous solution down the drain with plenty of water. The hydrolysis and neutralization reactions may generate heat and fumes which can be controlled by the rate of addition (14).

VIII. REFERENCES

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POTASSIUM PERCHLORATE (cont.)

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PROPYLENE GLYCOL 1,2-DINITRATE

Much of the available data on propylene glycol 1,2-dinitrate has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

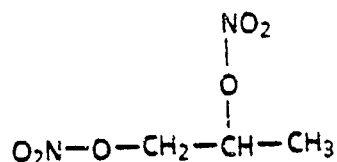
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_3H_6N_2O_6$

Molecular Weight: 166 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 6423-43-4

CA Name (9CI): 1,2-Propanediol, dinitrate

CA Name (8CI): Same

RTECS Number: TY6300000

Other significant synonyms: Isopropylene nitrate

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Colorless (1)

Odor: Disagreeable (1)

Boiling Point: 92°C at 10mm Hg (1)

PROPYLENE GLYCOL 1,2-DINITRATE (cont.)

Solubilities:

Water: Soluble in water (1)

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (specific gravity): 1.3774 (1)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: The glycol dinitrates hydrolyze rapidly in base, somewhat more slowly in acid and only at elevated temperatures in water alone. The hydrolysis of alkyl nitrates can lead to a variety of products including the parent alcohol, alkenes, aldehydes and carboxylic acids. Thermal decomposition of alkyl nitrates initially yields alkoxy radicals which react further to give complex mixtures which include CO, CO₂, NO_x. Photolysis also gives complex mixtures including NO (1).

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Principal constituent of Otto Fuel II for the Otto II torpedo (1).

B. Other Uses

No civilian uses (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Fine and Miles have developed a portable voltammeter to monitor nitrate esters, particularly PGDN in waste water using a silver wire electrode (2).

PROPYLENE GLYCOL 1,2-DINITRATE (cont.)

Erk et al. described a gas chromatography method using an electron capture detector to determine PGDN in blood (3).

B. Limit of Detection

Miles and Fine reported in their patent application that 0.5 mg/L is easily detectable (2).

Erk et al. claimed 10 ng/mL limit of detection by gas chromatograph (3).

PROPYLENE GLYCOL 1,2-DINITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF 1,2-PROPYLENE GLYCOL DINITRATE*

Species	Route	Dose/Duration	Effects	Reference
Human (workers exposed to 1,2-PGDN)	inhal- ation	Mean exposure duration: 47.4 or 91.8 mo	No significant differ- ences in mean scores of oculomotor and ataxia tests between exposed workers and controls	(5)
		Acute; peak conc. equal to or less than 0.1 ppm	Significant changes in oculomotor test scores	(5)
Guinea pig	intra- peritoneal	402 mg/kg	LD ₅₀	(6)
Rabbit	eye	100 mg	Mild irritation	(6)
Cat	subcu- taneous	200 mg/kg	LD _{LO}	(6)
Dog (Beagle)	intra- venous	4-100 mg/kg suspended in polyethylene glycol 400	Dose-related decreases in systolic, diastolic, and pulse blood pres- sure; dose-related in- crease in heart rate; whole red blood cells in urine; vasodilation; methemoglobinemia at high doses	(7)
Rhesus monkey	inhal- ation	0.3 ppm increasing to 4.23 ppm over 125 days	No significant changes in behavior or necropsy and histopathologic results	(8)
		2-33 ppm for 6 hr	No unequivocal changes in visual evoked response	(8)

* Information not included in the ARC report

PROPYLENE GLYCOL 1,2-DINITRATE (cont.)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

- A1. Transport -- Data not available
- A1a. Adsorption -- Data not available
- A1b. Volatilization -- Data not available
- A1c. Leachability -- Data not available
- A1d. Bioaccumulation -- Data not available
- A2. Transformation -- Data not available
- A2a. Biodegradation -- Data not available
- A2b. Hydrolysis -- Data not available
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available

B. Effects on animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available
- B7. Aquatic species, fish and invertebrates -- Data not available

C. Effects on plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

PROPYLENE GLYCOL 1,2-DINITRATE (cont.)

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (9).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (10).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Kitchens, J.F., S.G. Brownlee, W.E. Harward, III, R.G. Hyde, W.E. Jones, III, D.A. Price, R.S. Wentzel, and R.S. Valentine. 1979. Preliminary Problem Definition Study on Munitions-Related Chemicals. Final Report, ADA099733. Atlantic Research Corporation, Alexandria, VA. DAMD17-77-C-7057.
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PROPYLENE GLYCOL 1,2-DINITRATE (cont.)

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10. Forsten, I. 1980. Disposal of Hazardous Toxic Munition Waste. Proceedings of the 1980 National Conference of Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers Division, New York. 440-575.

PROPYLENE GLYCOL 1,3-DINITRATE

Much of the available data on propylene glycol 1,3-dinitrate has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_3H_6N_2O_6$

Molecular Weight: 166 (1)

Structural Formula: $O_3N(CH_2)_3NO_3$

B. Alternate Names and Registry Numbers

CAS Registry Number: 3457-90-7

CA Name (9CI): 1,3-Propanediol, dinitrate

CA Name (8CI): Same

RTECS Number: Data not available

Other Significant Synonyms: Trimethylene dinitrate

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Colorless (1)

Odor: Data not available

Boiling Point: $180^{\circ}C$ at 10 mm Hg (1)

Solubilities:

Water: Data not available

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Specific Gravity): 1.3952 (1)

PROPYLENE GLYCOL 1,3-DINITRATE (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: The glycol dinitrates hydrolyze rapidly in base, somewhat more slowly in acid and only at elevated temperatures in water alone. The hydrolysis of alkyl nitrates can lead to a variety of products including the parent alcohol, alkenes, aldehydes and carboxylic acids. Thermal decomposition of alkyl nitrates initially yields alkoxy radicals which react further to give complex mixtures which include CO, CO₂ and NO. Photolysis also gives complex mixtures including NO_x (1).

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Explosive and plasticizer (1).

B. Other Uses

None found

III. ANALYTICAL METHODS

A. Best Acceptable Method

No analytical methods were found in a computerized search of Chemical Abstracts dating back to 1967. Several methods were found for the 1,2-ester, including voltammetric and gas chromatographic analyses. These methods could possibly be extended to this compound. See the report on propylene glycol 1,2-dinitrate.

B. Limit of Detection

Data not available

PROPYLENE GLYCOL 1,3-DINITRATE (cont.)

IV. HEALTH EFFECTS

No information other than that in the ARC report was located. See report on 1,2-propylene glycol dinitrate.

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of 1,3-propylene glycol dinitrate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation or, occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USTHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (2).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (3).

C. Other Disposal Practices Employed

Data not available

PROPYLENE GLYCOL 1,3-DINITRATE (cont.)

VIII. REFERENCES

1. Kitchens, J.F., S.G. Brownlee, W.E. Harward III, R.G. Hyde, W.E. Jones, III, D.A. Price, R.S. Wentzel, and R.S. Valentine. 1979. Preliminary Problem Definition Study On Munitions Related Chemicals. Final Report, AD A099733. Atlantic Research Corporation, Alexandria, VA. DAMD17-77-C-7057.
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RED PHOSPHORUS

The Army's need for research on the toxicological and environmental hazardous of red phosphorus is defined in the Atlantic Research Corporation (ARC) report entitled, A Preliminary Problem Definition Study of 48 Munitions Related Chemicals. The report states that red phosphorus is considered relatively non-toxic to mammals unless it contains some of the white form, and that there is no evidence that the compound is toxic to aquatic life.

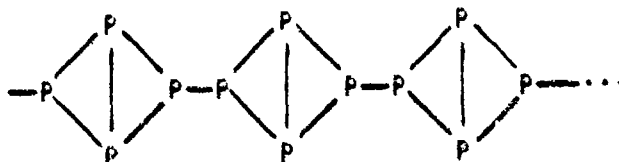
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: P_4

Molecular Weight: 123.92 (1) 124.08 (2)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 7723-14-0

CA Name (9CI): Phosphorus

CA Name (8CI): Phosphorus

RTECS Number: TH3495000

Other Significant Synonyms: Amorphous, red (2), phosphorus (3)

C. Chemical and Physical Properties

Physical State: Reddish-brown powder (2)

Color: Red to violet (4)

Odor: Data not available

RED PHOSPHORUS (cont.)

Melting Point: Sublimes at 416°C (5)

Boiling Point: 280° (6)

Solubilities:

Water: Insoluble

Nonaqueous Solvents: Insoluble in caustic alkali, carbon bisulfide, ether and ammonia solution (1). Insoluble in organic solvents, soluble in phosphorous tribromide (4).

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Data not available

Density (Crystal): 2.34 g/cc

Volatility: Data not available

Vapor Pressure: 0.181 torr at 25°C (6)

Vapor Density: 4.77 g/L

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Reacts only at high temperature; less reactive than white phosphorus (4). Avoid contact with potassium chlorate, potassium permanganate, peroxides and other oxidizing agents (4).

Flammability: Catches fire when heated in air to about 260° (autoignition temperature) and burns with formation of pentoxide. Burns when heated in an atmosphere of chlorine (4).

Ignition Point: 200°C (1)

Autoignition Temperature: 260°C in air (7)

II. USES

A. Army Unique Use

Obscurant, pyrotechnic (5)

B. Other Uses

Manufacture of phosphoric acid (q.v.) and other phosphorous compounds, phosphor bronzes, metallic phosphides, additive to semiconductors, electroluminescent coatings, incendiaries, safety matches, fertilizers (7).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Phosphorus can be detected in trace amounts by atomic emission spectrometry. Hee et al. have recently reported a simultaneous inductively coupled plasma atomic emission spectrometric method for phosphorus and 33 other elements (8).

A photometric detector for gas chromatography, designed to monitor cold chemiluminescence has been reported by Mielniczuk (9).

B. Limit of Detection

Hee et al. reported a lowest quantifiable limit (LQL) of less than 0.1 microgram per milliliter (8).

RED PHOSPHORUS (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF RED PHOSPHORUS*

Species	Route	Dose/Duration	Effects	Reference
Human	NS**	4,412 ug/kg	LD ₁₀	(10)
Human	NS	NS	Relatively nontoxic unless it contains white phosphorus as an impurity	(4)
Human	NS	NS	Irritant to eyes	(11)
Human	Inhalation	40 mg/m ³	Acu. atypical pneumonia of sudden onset as observed in workers in plants producing red phosphorus by sublimation of white phosphorus	(12)
Human	Inhalation	100-700 mg/m ³ for less than 15 min	Phosphorus smoke formulations caused reversible pulmonary symptoms and mucous membrane irritation	(12)
F344 Rat	Oral	>10,000 mg/kg	LD ₅₀	(13)
Rat	Inhalation	1,537 mg/m ³ /1 hr	Smoke caused mortality of 1/10	(12)
		1,676 mg/m ³ /2 hr	Smoke caused mortality of 4/10	
		1,572 mg/m ³ /3 hr	Smoke caused mortality of 8/10	

* Information not included in the ARC Report.

** Not specified.

RED PHOSPHORUS (cont.)

TABLE IV-1. TOXICITY OF RED PHOSPHORUS (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Porton rat and New Zea- land rabbit	Inhal ation	6,700-6,800 ppm/30 min	Smoke of two pyrotechnic mixtures containing 95% red phosphorus plus 5% butyl rubber or 97% red phosphorus plus 3% butadiene styrene caused inflammation and epithelial necrosis of the larynx and trachea, alveolitis, and broncho-pneumonia. The effects were attributed to pyrolytic production of ortho phosphoric acid	(14)
New Zealand rabbit	Eyes	100 mg dry material in one eye	No irritation	(13)
New Zealand rabbit	Intact and abraded skin	500 mg/L/in ² / 24 h	No irritation	(13)
Female Hartley Guinea pig	Inhal- ation	352 ppm/10 min 800 ppm/10 min	Smoke caused mortality of 4/10 Smoke caused mortality of 9/10	(12)
Female Hartley Guinea pig	Intra- dermal	0.1 mL of a 1 g/L solution 3 x w for 10 doses	Slight irritation but no sensitization	(13)
Female Hartley Guinea pig	Skin	0.5 mL of a 100 g/L sol- ution 6 h/3x w for 10 doses	No sensitization	(13)

* Information not included in the ARC report.

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF RED PHOSPHORUS

Test System	Dose	Effects	References
<u>S.typhimurium</u> TA100, TA1535, TA1537, TA1538	NS*	Not active with or without Aroclor 1254-induced rat liver S9	(15)
<u>S. cerevisiae</u>	NS	Not active with or without Aroclor 1254-induced rat liver S9	(15)
<u>E. Coli</u> W3110/poA ⁺ , p3478/poA ⁻	100 ug- 10 mg	Not active with or without Aroclor 1254-induced rat liver S9	(15)
** Not specified			

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of red phosphorus which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Red phosphorus is excluded from designation as hazardous in that it is a nontoxic allotrope, although it is frequently contaminated with a small amount of the yellow (16).

B. Environmental

Reported in EPA TSCA Inventory 1983.

Phosphorus has a statutory reportable quantity (RQ) of 1 lb. under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (17).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

A recent programmatic life cycle environmental assesment indicates that incineration is the preferred method for disposal of smoke/obscurant munitions. Munitions containing phosphorous would be incinerated in a unit equipped with afterburner and a scrubber (18).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Controlled incineration followed by alkaline scrubbing and particulate removal equipment (17).

Cautiously make a 5% solution of the product in water; vent because of possible vigorous evolution of flammable hydrogen gas. Acidify the solution to pH 1 by adding 1M sulfuric acid dropwise. Acidification will cause vigorous evolution of hydrogen gas. Allow the solution to stand overnight. Evaporate to dryness and bury the residue in a chemical landfill (19).

VIII. REFERENCES

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RED PHOSPHORUS (cont.)

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SODIUM AZIDE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: NaN_3

Molecular Weight: 65.02 (1)

Structural Formula: $\text{Na}^{+1}(\text{N}=\text{N}=\text{N})^{-1}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 26628-22-8

Deleted CAS Registry Numbers: 20828-18-6; 12136-89-9

CA Name (9CI): Sodium azide NaN_3

CA Name (8CI): Sodium azide

RTECS Number: VY8050000

Other Significant Synonyms: Smite

C. Chemical and Physical Properties

Physical State: Crystal (1) hexagonal (2)

Color: Colorless (2)

Odor: Data not available

Melting Point: Decomposes to nitrogen and sodium (1)

Solubilities:

Water: 40.16% at 10°C (1); 41.7% at 17°C (1)

Nonaqueous Solvents: 0.3% in alcohol at 25°C (1). Insoluble in ether; soluble in liquid ammonia (1).

Octanol Water Partition Coefficient: Not applicable

Hygroscopicity: Data not available

Density (Crystal): 1.846 g/cc (2)

SODIUM AZIDE (cont.)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Moderate (3)

II. USES

A. Army Unique Use

Data not available

B. Other Uses

In the preparation of hydrazoic acid, lead azide, and pure sodium; as a propellant for inflating automotive safety bags; and in weed and fruit rot control (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

Misovets (4) reported a thin-layer chromatography system for the detection of sodium azide, using Silufol plates and 40:20:1 acetone:water:formic acid mobile phase and 0.2% ninhydrin solution in butyl alcohol as the visualizing agent. Asplund (5) reported a voltammetric determination of sodium azide in trace amounts from air using a dropping mercury electrode.

B. Limit of Detection

Misovets (4) reported 0.01-0.1 mg; Asplund (5) reported 0.05 mg per cubic meter.

SODIUM AZIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF SODIUM AZIDE

Species	Route	Dose/Duration	Effects	References
Human	NS *	Acute	Hypotension (unresponsive to pressor drugs), tachycardia, tachypnea, hypothermia, acidosis, convulsions, severe headache	(6)
Human	NS	0.2-4.0 ug/kg	Extremely potent directly acting vasodilator	(6)
Human	oral	"Several g"	Collapse and death within 40 min; swelling of the brain and lungs; mild fatty degeneration of the liver	(6)
Human	oral	50-60 mg	Collapse within 5 minutes accompanied by hypotension and tachycardia lasting almost 1 hr	(6)
Human	oral	150 mg (in aqueous solution)	Breathlessness and tachycardia within 5 min; nausea, vomiting, headache, restlessness, and diarrhea within 15 min; later polydipsia, ECG changes, and leukocytosis occurred	(6)
Human	oral	710 ug/kg	Behavioral and urogenital symptoms	(7)
Human	oral	0.01-0.02 mg/kg	A drop in blood pressure for 10 to 15 min in hypertensive patients	(8)
Human	inhalation	NS	Vapor and fumes are irritants of mucous membranes; heavy exposure has caused bronchitis and pulmonary edema	(6)

* Not specified

SODIUM AZIDE (cont.)

TABLE IV-1. TOXICITY OF SODIUM AZIDE (Cont.)

Species	Route	Dose/Duration	Effects	References
Rat	oral	42 mg/kg	LD _{Lo}	(7)
Rat	oral	2,730 or 5,460 mg/kg, total dose, 78 wk	Equivocal evidence for tumors of the endocrine system and skin	(7)
Rat	oral	27 mg/kg	LD ₅₀	(7)
Rat	intra- peri- toneal	30 mg/kg	LD _{Lo}	(7)
Rat	intra- peri- toneal	5-10 mg/kg, 2-4x/hr for 3-6 hr	Severe intoxication; some survivors show injury and demyelination of myelinated nerve fibers in the central nervous system and testic- or kidney lesions	(8)
Rat	sc	35 mg/kg	LD _{Lo}	(7)
Mouse	oral	27 mg/kg	LD ₅₀	(7)
Mouse	intra- peri- toneal	18 mg/kg	LD ₅₀	(7)
Mouse	intra- venous	19 mg/kg	LD ₅₀	(7)
Rabbit	oral	3-10 mg/kg	40-60% reduction in blood pressure lasting over 1 hr	(8)

TABLE IV-1. TOXICITY OF SODIUM AZIDE (Cont.)

Species	Route	Dose/Duration	Effects	References
Monkey	NS*	Repeated doses	Central nervous system effects: blindness and attacks of rigidity with abnormal motions	(8)

DAMD17-84-C-4133

50-4

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF SODIUM AZIDE*

Test System	Dose	Effects
<u>Salmonella</u> <u>typhimurium</u>	3 mmol/L/ 2 hr	Mutagenic
<u>S. typhimurium</u>	1 ug/ plate	Mutagenic with metabolic activation
<u>Escherichia</u> <u>coli</u>	150 nmol/L	Mutagenic
<u>E. coli</u>	5 gm/L	Effects on DNA repair
Insect	100 mg/L oral	Dominant lethal mutation and heritable translocation
Human fibro- blasts	50 mg/L	DNA synthesis inhibition
Rat liver cells	1 mmol/L	Mutagenic
Mouse lymphocytes	500 mg/L/ 2 hr	Mutagenic
Hamster lung cells	1 mmol/L	Effects on DNA repair

* Data from RTECS (1985)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

Ala. Adsorption -- Data not available

Alb. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

SODIUM AZIDE (cont.)

- A2a. Biodegradation -- Data not available
- A2b. Hydrolysis -- In water, sodium azide will shift between the dissolved salt form and hydrazoic acid depending upon solution pH. Azides react with many organics to form amines. They can also be oxidized to nitrates or reduced to ammonia. The azide ion itself will not persist in solution (9).
- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available
- B. Effects on animals
- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Sodium azide impairs the phototaxis (light-orienting capability) of the photosynthetic flagellate alga, Euglena gracilis (10).
- B7. Aquatic species, fish and invertebrates -- Threshold toxicities in river water: Daphnia: 0.3 ppm; Microregma: 3.0 ppm; Scenedesmus: 4.0 ppm; Escherichia coli: 19.0 ppm (9).

Fish: 50% inhibition of carbonic anhydrase activity from the red blood cells of Ictalurus punctatus at 5900 ug/L sodium azide (11).

Crustacean: Gammarus lacustris: 24-hour LC_{50} : 14000 ug/L; 48-hour LC_{50} : 9000 ug/L; 96-hour LC_{50} : 5000 ug/L. (12).

- C. Effects on plants
- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available

SODIUM AZIDE (cont.)

- C3. Metabolism -- Sodium azide inhibits the two photosynthesis partial reactions of 3-phosphoglycerate photoreduction and oxaloacetate photoreduction, as demonstrated by study in permeabilized cell preparations from wild type and mutants of Chlamydomonas reinhardtii (13).

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1980.

Sodium azide has a statutory reportable quantity (RQ) of 1 lb. under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the RQ (14).

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

AEHA: NSN 6810-00-300-3423

a. Dispose of through a commercial contractor.

b. Dispose of using a special procedure.

Detonation of this item shall be accomplished by Explosive Ordnance Disposal (EOD) experts only at a remote uninhabited location. The U.S. Army Escort Unit, if requested, is available to assist in the disposal of this item. AR 740-32 outlines the procedure necessary to obtain their services. Liaison may be established with their Disposal Office, AUTOVON 584-4382. EOD personnel shall determine the amount to be disposed of at a given time in accordance with their Range Safety and Movement Regulation. Movement of this material from a storage location to a range for disposal shall be in accordance with existing Department of Transportation regulations as well State and local regulations (15).

SODIUM AZIDE (cont.)

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

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SODIUM PERCHLORATE

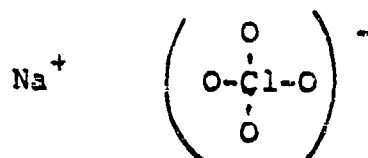
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: NaClO_4

Molecular Weight: 122.44

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 7601-89-0

CA Name (9CI): Perchlorate acid, sodium salt

CA Name (8CI): Perchlorate acid, sodium salt

RTECS Number: SC 9800000

Other Significant Synonyms: Irenat (1)

C. Chemical and Physical Properties

Physical State: Deliquescent crystals (2)

Color: White

Odor: Odorless (3)

Melting Point: Decomposes at 482°C (4).

Solubilities:

Water: Very soluble (2)

Nonaqueous Solvents: 51.4 g/100g methyl alcohol; 51.7 g/100g acetone; 14.7 g/100g ethyl alcohol; 4.89 g/100g propyl alcohol; 1.86 g/100g butyl alcohol; 9.65 g/100g ethyl acetate; 0.786 g/100g iso-butyl alcohol; insoluble in ether (5).

SODIUM PERCHLORATE

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Deliquescent

Density (Crystal): Specific Gravity: 2.02 (2)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: A powerful oxidizing agent, readily combustible if mixed with organic material (6). Pure NaClO_4 is insensitive to impact (5). Strong oxidant when heated, particularly under acidic conditions. Forms an explosive with ammonium nitrate, calcium hydride, charcoal, magnesium, strontium hydride and with reducing agents (1).

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Explosives, pyrotechnics

B. Other Uses

Jet fuel, analytical reagent (2)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Sodium can be determined by atomic absorption or by atomic emission spectrometry as described by Hee (7).

A perchlorate membrane selective electrode has been developed, but it may not be sensitive for trace analysis. Khokhlova et al. have used this electrode to study activity coefficients of perchlorate ions (8).

B. Limit of Detection

Hee reports a lower determination range of 0.01-0.1 ug/ml for sodium (7).

SODIUM PERCHLORATE

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF SODIUM PERCHLORATE

Species	Route	Dose/Duration	Effects	Reference
Human	oral	Therapeutic dose levels	Nausea, vomiting, and hypersensitivity reactions such as maculopapular rashes, fever, and lymphadenopathies may occur; fatal aplastic anemia has occurred in a small proportion of patients; agranulocytosis, thrombocytopenia, and leucopenia have been reported; antithyroid activity	(3)
Human	contact with dust	NS*	Irritation of skin, throat, eyes, and nose	(5)
Rat	oral	2,100 mg/kg	LD ₅₀ ; effects on behavior, pulmonary system, metabolism	(9)
Rat	intra-peritoneal	20 mg	Antithyroid activity	(10)
Mouse	intra-peritoneal	551 mg/kg	LD ₅₀	(9)
Rabbit	injection	aqueous solution; conc. and duration NS	No long term toxic effects; "behaved as a mild muscular poison"; large doses produced diarrhea and liver damage	(5)

*Not specified

SODIUM PERCHLORATE

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF SODIUM PERCHLORATE

Test System	Dose	Effects	Reference
<u>E. coli</u> DNA repair assay	1500 pmol/ plate	Active	(9)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

A2a. Biodegradation -- A few microorganisms are able to metabolize perchlorate; most are not. It has been reported that perchlorate is reduced to chloride by several species of heterotrophic bacteria, including the very common E. coli and Pseudomonas aeruginosa. Some Streptococcus and Flavobacterium spp. were inactive (11).

A2b. Hydrolysis -- Data not available

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Data not available

A2e. Half-life -- Data not available

B. Effects on animals

B1. Avian species -- Data not available

B2. Mammalian wildlife species -- Data not available

B3. Terrestrial invertebrates -- Data not available

B4. Reptiles -- Data not available

SODIUM PERCHLORATE

- B5. Amphibians -- The acute toxic level of sodium perchlorate to tadpoles is reported to be 2000 mg/L. Chronic effects appear at much lower levels. Newts maintained at a level of 36 mg/L of perchlorate exhibit significant histological changes in the thyroid and pituitary. Continuous exposure to 360 mg/L results in arrested metamorphosis in tadpoles and a grossly enlarged thyroid in guppies (11).
- B6. Microorganisms, aquatic and soil -- A 2% solution of sodium perchlorate will check the growth of E. coli; about 10% is required to check the growth of Staphylococcus aureus and Sterigmatocystis nigra (11). Sodium perchlorate added to incubated soil caused inhibition of the respiration activity and a decrease in the number of ammonifying, nitrifying and denitrifying bacteria. In pure cultures of soil bacteria, the reduction of NO_3^- to NH_4^+ , the reduction NO_3^- to NO_2^- , and NO_3^- utilization were inhibited. The ClO_4^- ions act in two ways: by liberating metabolites (Cl^-) toxic to the cells and by competing with NO_3^- for the nitrate reductase A enzyme (12).
- B7. Aquatic species, fish and invertebrates -- Although few definitive studies have been conducted, it appears that the acute toxicity of perchlorate ion to aquatic animals and microorganisms is very low, with toxic levels probably exceeding 1000 mg/L for periods of 24 hours and longer. Because perchlorate is an important antithyroid agent, chronic effects may appear at much lower levels (11).
- C. Effects on plants
- C1. Phytotoxicity -- Soybeans grown in water culture exhibit toxic symptoms at perchlorate levels as low as 2.5 mg/L four days after application. Soybeans grown in sand were noticeably less susceptible (11).
- C2. Uptake -- Uptake of iodide by the seaweed Fucus ceranoides is competitively inhibited by perchlorate at the 0.1 mg/L level in seawater (11).
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1983.

SODIUM PERCHLORATE

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (13).

- B. Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (14).

C. Other Disposal Practices Employed

Use vast volume of concentrated solution of reducing agent (bisulfites or ferrous salts with $3M-H_2SO_4$ or hypo). Neutralize with soda ash or dilute with HCl. Drain into a sewer with abundant water (6).

Bury in a landfill site approved for the disposal of chemical and hazardous waste (15).

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SODIUM PERCHLORATE

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STRONTIUM OXALATE

Much of the available data on strontium oxalate has been reported in a previous study by the Atlantic Research Corporation (ARC), entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

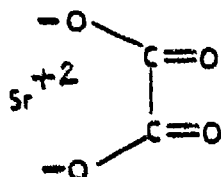
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{SrC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ (1)

Molecular weight: 193.64 (1)

Structural formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 814-95-9

Deleted CAS Registry Number: 14529-93-2

CA Name (9CI): Ethanedioic acid, strontium salt (1:1)

CA Name (8CI): Oxalic acid, strontium salt (1:1)

RTECS Number: Data not available

Other significant synonyms: Data not available

C. Chemical and Physical Properties

Physical State: Crystalline powder (1)

Color: Colorless (1)

Odor: Odorless (1)

Melting Point: 150 °C with loss of H_2O (1)

STRONTIUM OXALATE (cont.)

Solubilities:

Water: Slightly soluble (1), 1 in 20,000 parts water; 1 in 1900 parts of 3.5% acetic acid; 1 in 1115 parts of 23% acetic acid, but less soluble in 35% acetic acid; readily soluble in dilute HCl or HNO_3 (2).

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Hydrolyzes to form oxalic acid and strontium hydroxide.

Thermal decomposition proceeds with an initial loss of water, formation of strontium carbonate and finally formation of strontium oxide (1).

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Constituent of R-256 tracer mix used in the M-17, .50 caliber tracer rounds (1).

B. Other Uses

Radiator cleaner (1)

STRONTIUM OXALATE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

No methods have been developed to analyze strontium oxalate as a complete entity since the publication of the ARC report. Newer methods have been developed for the analysis of strontium such as simultaneous inductively coupled plasma atomic emission spectrometry as reported by Hee et al. (3).

B. Limit of Detection

Hee et al. reported a lower determination limit range for strontium as $<0.001 \text{ ug/mL}$ (3).

STRONTIUM OXALATE (cont.)

IV. HEALTH EFFECTS

TOXICITY OF STRONTIUM OXALATE*

Chemical	Route	Effects	Reference
Strontium oxalate		No toxicity data located; data on chemical classes follow below	
Strontium Salts	oral, inhalation	Moderately irritating; the strontium ion has a low order of toxicity	(4)
Oxalates	oral, inhalation	High acute toxicity	(4)
	local	Powerful irritant; corrosive to tissue; when taken by mouth, oxalates produce a caustic effect on the mouth, esophagus, and stomach	(4)

* Information not included in the ARC report

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of strontium oxalate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory.

STRONTIUM OXALATE (cont.)

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

A recent programmatic life cycle environmental assessment indicates that incineration is the preferred method for disposal of smoke/obscurant munitions. Munitions containing strontium oxalate should be incinerated in a unit equipped with afterburner and a scrubber; scrubber overflow should be neutralized prior to discharge (5).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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TETRANITROCARBAZOLE

Much of the available data on tetranitorcarbazole has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

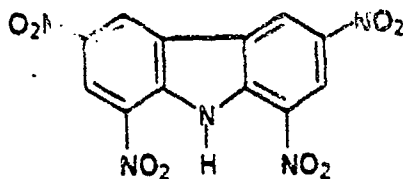
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{12}H_5N_5O_8$

Molecular Weight: 347.2 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 4543-33-3

CA Name (9CI): 9H-Carbazole, 1,3,6,8-tetranitro

CA Name (8CI): Carbazole, 1,3,6,8-tetranitro

Alternate CAS Registry Number: 28453-24-9

Alternate CA Name (9CI): 9H-Carbazole, tetranitro

Alternate CA Name (8CI): Carbazole, tetranitro

RTECS Number: Not listed in RTECS

Other Significant Synonyms: TNC

C. Chemical and Physical Properties

Physical State: Powder (1)

TETRANITROCARBAZOLE (cont.)

Color: Yellow (1)

Odor: Data not available

Melting Point: 285°C (1)

Solubilities:

Water: Insoluble (1)

Nonaqueous Solvents: Soluble in hot acetone (1). Soluble in benzene; insoluble in ether, alcohol and chloroform (2).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Not hygroscopic (2)

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: 3773 cal/g (1)

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

TNC is a constituent in a yellow first-fire mixture that is used to ignite the primary explosive charge (1).

B. Other Uses

Less than 25 pounds per year consumed for civilian purposes. Formerly used in fireworks (1). Compound has been cited in a Japanese patent and 1,3,6,7-TNC specifically for use in electrophotographic photosensitive plates (3).

III. ANALYTICAL METHODS

No analytical methods were reported in Chemical Abstracts in a computerized search of both registry numbers, dating back to 1967.

TETRANITROCARBAZOLE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. HEALTH EFFECTS RELATED TO TETRANITROCARBAZOLE*

Chemical	Effects	References
Tetranitrocarbazole	Unknown, probably toxic	(4)
Organic nitrates and nitrites	Vasodilation, headache, dizziness, weakness, and other signs of cerebral ischemia associated with postural hypotension; large amounts may produce coma, convulsions, and collapse	(5)
<u>Data On Analogues</u>		
2,4,7-Trinitro-9-fluorenone**	Carcinogenic and mutagenic	(6)
2,7-Dinitrofluorene**	Carcinogenic and mutagenic	(6)

* Information not included in the ARC report

** Structurally related to tetranitrocarbazole

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of tetranitrocarbazole that updates the ARC report.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

TETRANITROCARBAZOLE (cont.)

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Review of past Installation Assessment Reports indicates that current methods of disposal of waste explosives and propellants involve open burning, open detonation, or occasionally, hauling by a licensed contractor and landfilling. Current use of methods discussed above has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices and to develop plans for future disposal practices (7).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (8).

C. Other Disposal Practices Employed

Small Spill: Absorb or sweep on paper. Burn in iron pan in fume hood.

Large Spill: Mix with sand. Package in paper carton. Transfer to sanitary landfill. Wash spill site with strong soap and water (4).

VIII. REFERENCES

1. Kitchens, J.F., S.G. Brownlee, W.E. Harward, III, R.G. Hyde, W.E. Jones, III, D.A. Price, R.S. Wentzel, and R.S. Valentine. 1979. Preliminary Problem Definition Study on Munitions-Related Chemicals. Final Report, AD A099733. Atlantic Research Corporation, Alexandria, VA. DAMD17-77-C-7057.
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TETRANITROCARBAZOLE (cont.)

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TETRYL

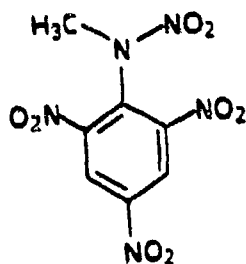
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_7H_5N_5O_8$

Molecular Weight: 287.17

Structural formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 479-45-8

CA Name (9CI): Benzenamine, N-methyl-N,2,4,6-tetranitro-

CA Name (8CI): Aniline, N-Methyl-N,2,4,6-tetranitro-

RTECS Number: BY6300000

Other Significant Synonyms: Nitramine; Tetralite; Tetril; 2,4,6-Tetryl;
Trinitrophenylmethylnitramine; 2,4,6-Trinitrophenylmethylnitramine

C. Chemical and Physical Properties

Physical State: Monoclinic crystals

Color: Yellow

TETRYL (cont.)

Odor: Data not available

Melting Point: 130-132 °C

Boiling Point: 180-190 °C

Solubilities:

Water: Insoluble (1)

Nonaqueous Solvents: Soluble in alcohol, ether, benzene, glacial acetic acid (1).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): 1.57 g/cc (1)

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: $0.0523 + 6.62 \times 10^{-4} T$ cal/g/°C

Heat of Combustion: 2,925 kcal/kg (2)

Reactivity: Severe explosive hazard when shocked or exposed to heat or flame. Sensitive to percussion (3). Dangerous fire risk (4). Highly resistant to attack by dilute mineral acids (5). Does not react with aluminum, tin, copper, nickel lead or Cu-plated steel, bronze and stainless steel (5).

Vapor Density: 9.92 g/cc

Stability: Fairly resistant to gamma radiation (6).

Heat of Combustion: 2,925 cal/g (6)

Flammability: Autoignition temp = 166°C; explosive temperature = 257°C. Explodes at 180 to 190 °C (7).

II. USES

A. Army Unique Use

High explosive

B. Other Uses

Acid-base indicator; pH 10.8 colorless; pH 13.0 reddish brown (1).

TETRYL (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Several chromatographic methods are reported in the recent literature. Lloyd reported a high performance liquid chromatography method that used a pendant mercury drop electrode at the detector. This method compares favorably with electron capture detection in gas chromatography (8).

A thermal energy analyzer (TEA) interfaced with a gas or liquid chromatograph was reported by Fine (9) to detect explosive in debris without prior clean-up.

Cantu et al (10) reported success using a Fourier transform infrared spectrometer coupled with HPLC.

Yinon (11) described a custom built mass spectrometer interfaced with an HPLC that can successfully analyze tetryl and other explosives.

Malotky and Downes (12) reported a field kit for the analysis of 28 different explosives including tetryl using thin-layer chromatography.

B. Limit of Detection

Lloyd (8) reported a detection limit of 2-20 picogram/10 microliters of injected sample.

Fine (9) reported a detection limit of <10 picograms.

TETRYL (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF TETRYL

Species	Route	Dose/Duration	Effects	Reference
Human	inhal- ation skin and eye	NS*	Potent sensitizer causing allergic dermatitis. Severe cases show massive generalized edema with partial obstruction of the trachea. Acutely irritating to the mucous membranes of the respiratory tract and eyes causing coughing, sneezing, epistaxis, conjunctivitis, and palpebral edema. Systemic effects include irritability, easy fatigability, malaise, headache, lassitude, insomnia, nausea, and vomiting. Anemia of both the marrow depression or deficiency type.	(13)
Human	occupa- tional exposure	NS	Powerful sensitizer causing dermatitis. Local irritation of the conjunctiva, nose, throat and bronchial tubes, producing common cold-like symptoms, nose bleed, cough, and occasionally asthma-like symptoms. No reports of systemic or internal poisoning.	(14)
Human	inhal ation skin	NS	Gastrointestinal symptoms and anemia may develop. May cause tracheitis and asthma.	(15)
Rat	oral (route implied)	1 g/kg daily up to 3 mo	Necrosis of the liver and degeneration of the kidney	(16)

TETRYL (cont.)

TABLE IV-1. TOXICITY OF TETRYL (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Dog	sc	5,000 mg/kg	LD _{Lo}	(17)

* Not specified

TABLE IV-2. CARCINOGENICITY OF TETRYL

Species	Route	Dose/Duration	Effects	Reference
Female Sprague- Dawley rat	oral	10 doses of 40 mg/rat at 3-d intervals; observed for 9 mo	No effect, but study is inadequate	(18)

TETRYL (cont.)

TABLE IV-3. MUTAGENICITY AND RELATED EFFECTS OF TETRYL

Test System	Dose	Effects	Reference
<u>Salmonella</u> <u>typhimurium</u> TA98, TA100 TA1537, TA1538	33.3 or 100 ug/ plate	Mutagenic with and without Aroclor 1254- induced rat liver S9.	(19)
<u>Saccharomyces</u> <u>cerevisiae</u> D5	62.5 and 125 ug/ml	Increased frequency of mitotic recombination in the absence of Aroclor 1254-induced rat liver S9. Not active with S9.	(19)
<u>S. typhimurium</u> TA100, TA1535	5 ug/plate	Analytical-grade: muta- genic in TA100 and TA1535. Military-grade: mutagenic in TA100 but less so than analytical-grade	(20)
<u>S. cerevisiae</u> D4	5 ug/plate	Mutagenic causing mitotic gene conversions at ade and trp.	(20)
<u>Neurospora</u> <u>crassa</u>	10 ug/ plate	Mutagenic inducing ad-3 ⁺ reversions.	(20)

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- A six-month study showed very little detectable movement of tetryl or its transformation products through soil columns in that time frame. This may be combined result of soil fixation and limited water solubilities of the compounds (21).

A1b. Volatilization -- Data not available

A1c. Infiltration -- Data not available

A1d. Bioaccumulation -- Data not available

A2. Transformation -- Data not available

TETRYL (cont.)

- A2a. Biodegradation -- Biodegradation in 7 day tests: nil % degradation in original culture, neither in 1st, 2nd or 3rd subculture (22).
- A2b. Hydrolysis -- In natural waters tetryl is slowly degraded to picric acid. Authors recovered no information indicating that wastewater effluents containing picric acid or its metabolite, picramic acid, in concentrations anticipated from the degradation of tetryl, would present an environmental hazard, either directly or indirectly (23). The principal detectable product of the hydrolysis of tetryl in the dark, in borax buffer, is methylnitramine. Other identified products include: picrate ion, nitrite ion, N-methylpicramide, and nitrate ion. In a 110-day test, no degradation of the methylnitramine was noted (24).
- A2c. Photolysis -- Tetryl photolyzes under ambient lighting conditions at least an order of magnitude faster than it hydrolyzes. The major photoproduct is N-methylpicramide (trinitromethylaniline) (24).
- A2d. Other chemical reaction -- Tetryl reacts in concentrated sulfuric acid to form N-methylpicramide (24).
- A2e. Half-life -- The hydrolysis half-life of tetryl was estimated for a range of activation energies, for environmental conditions of 20°C and pH 6.8, to be approximately equal to 302 days (plus or minus 76 days). The author notes that some soils might have a strong accelerating effect on tetryl's hydrolysis rate which could drastically alter its environmental hydrolysis half-life (24).

B. Effects on Animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available
- B7. Aquatic species, fish and invertebrates -- Data not available

C. Effects on Plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available

TETRYL (cont.)

C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 1.5 mg/cu m (skin) (25)
STEL 3.0 mg/m³ (skin) (25)
PSHA-air: TWA 1500 ug/m³ (Skin) (26)
DGT-class A explosive (27)
Tentative STEL value: 3.0 mg/m³ (28)

B. Environmental -- Data not available

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (31).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (32).

C. Other Disposal Practices Employed

Pour into sodium bicarbonate or a mixture of sand-soda ash (9:1). After mixing, transfer into a paper carton filled with packing paper. Burn in an open furnace, or more efficiently, in a furnace with afterburner and scrubber (4).

Tetryl can be decomposed by heating it with an aqueous sodium sulfide solution. (Reference provides specific procedure). Supernatant liquid is discharged to a sump and any precipitate is burned in a burning ground (29). Activated carbon with regeneration capacity was recommended system for removal of tetryl among other compounds from munitions wastewater, in a study which compared carbon and polymeric resin adsorbents for this purpose (30).

TETRYL (cont.)

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TITANIUM TETRACHLORIDE

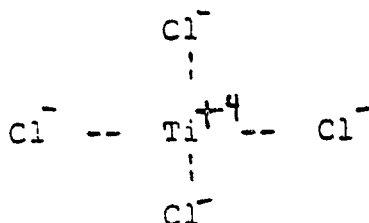
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: TiCl_4 (1)

Molecular Weight: 189.73 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 7550-45-0

Deleted CAS Registry Numbers: 44246-22-2, 15612-71-2

CA Name (9CI): Titanium chloride (TiCl_4)

CA Name (8CI): Titanium chloride (TiCl_4)

RTECS Number: XR1925000

Other Significant Synonyms: Tetrachlorotitanium

C. Chemical and Physical Properties

Physical State: Liquid (1)

Color: Colorless (1); light yellow (2)

Odor: Penetrating acid odor (1)

Melting Point: -24.1°C (1)

TITANIUM TETRACHLORIDE (cont.)

Boiling Point: 136.4°C (1)

Solubilities:

Water: Soluble in cold water, decomposed by hot water (1), soluble in dilute HCl (2).

Nonaqueous Solvents: Soluble in alcohol

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Hygroscopic (1)

Specific Gravity: 1.726

Volatility: Volatile, adsorbs moisture through the air and evolves dense white fumes (1).

Vapor Pressure: 100 mm at 91°C (3), 11.7 mm at 25°C

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Reactive only under extreme conditions (3).

Stability: Data not available

Flammability: Nonflammable (3)

II. USES

A. Army Unique Use

Smoke agent "FM" (4)

B. Other Uses

Formerly used with potassium bitartrate as a mordant in textile industry, and with dyewoods in dyeing leather; also as smoke-producing screen with ammonia and in the manufacture of iridescent glass and artificial pearls (1).

Laundering; chemical production; and in chemical laboratories (3).

TITANIUM TETRACHLORIDE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

Titanium can be determined through atomic absorption or atomic emission spectrometry (AES). Hee reported a simultaneous inductively coupled plasma AES method for determining titanium and 33 other elements.

B. Limit of Detection

Hee reported a lower determination limit range for titanium as <0.001 microgram/milliliter.

TITANIUM TETRACHLORIDE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF TITANIUM TETRACHLORIDE

Species	Route	Dose/Duration	Effects	Reference
Human	ingestion	NS*	Nausea, vomiting, cramps, diarrhea, and possible tissue ulceration	(6)
Human	contact with liquid	NS	Thermal and acid burns of eyes, skin, throat, and stomach; lasting deep brown pigment about the periphery of the scars and in areas of healed burns	(6)
Human	contact with vapor	NS	Severe irritation and damage to eyes, coughing, headache, dizziness, lung damage, and bronchial pneumonia	(7)
Human	inhalation	Approx. 2 min after industrial accident	Pulmonary burns followed by diffuse endobronchial polyp formation	(8)
Human	NS	NS	Late development of upper respiratory and nervous system disturbances	(6)
Rat	inhalation	460 mg/m ³ /4 hr	LC ₅₀	(9)
Mouse	inhalation	10 mg/m ³ /2 hr	LC _{Lo}	(9)
Guinea pig (albino)	skin	2x/d for 3d (liquid)	Destruction of the outer layers of the skin comparable to a second-degree thermal burn	(7)

TITANIUM TETRACHLORIDE (cont.)

TABLE IV-1. TOXICITY OF TITANIUM TETRACHLORIDE (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Dog	inhalation	intermittent exposures of 1-2 hr; conc. not measured	Respiratory distress with vomiting; decreased blood pressure, increased pulse and respiration rate; focal congestion and hemorrhage of the lungs with particulate deposits of Ti in the alveoli; mortality due to intense bronchitis and some edema interpreted as HCL effects	(7)
Dog	inhalation	6 hr/d, 5 d/wk, 9 wk; conc.: 8.4 ppm Ti, 6.8 ppm volatile chloride	No weight loss; increased leukocyte count; lung foci consisting of monocytes with brown Ti granules grouped around the bronchi and necrotic cells associated with proliferation of connective tissue	(7)

* Not specified

V. ENVIRONMENTAL EFFECTS

A. Environmental Fate

A1. Transport -- Data not available

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

1d. Bioaccumulation -- Concentration factors of 200 to 10,000 for 6 species of brown algae are reported; invertebrates, 2000; fish, 1000 (3).

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- Reacts vigorously with water to evolve HCl gas and $Ti(OH)_4$ (3).

TITANIUM TETRACHLORIDE (cont.)

- A2c. Photolysis -- Data not available
- A2d. Other chemical reaction -- Data not available
- A2e. Half-life -- Data not available
- B. Effects on animals
 - B1. Avian species -- Data not available
 - B2. Mammalian wildlife species -- Data not available
 - B3. Terrestrial invertebrates -- Data not available
 - B4. Reptiles -- Data not available
 - B5. Amphibians -- Data not available
 - B6. Microorganisms, aquatic and soil -- Data not available
 - B7. Aquatic species, fish and invertebrates -- Median threshold effect:
Scenedesmus: 96-hour test, 2 ppm as titanium; Daphnia: 48-hour test,
4.6 ppm as titanium; Microregma: 48-hour test, 4 ppm as titanium (3).
- C. Effects on plants
 - C1. Phytotoxicity -- Toxic to sugar beets at 12 ppm as titanium (3).
 - C2. Uptake -- Data not available
 - C3. Metabolism -- Data not available
- VI. STANDARDS AND REGULATIONS
 - A. Health
Data not available
 - B. Environmental
Data not available

TITANIUM TETRACHLORIDE (cont.)

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

A recent programmatic life cycle environmental assessment indicates that incineration is the preferred method for disposal of smoke/obscurant munitions (10). Munitions containing titanium tetrachloride should be incinerated in a unit equipped with afterburner and a scrubber; scrubber overflow should be neutralized prior to discharge.

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Sift or pour onto a dry layer of sodium bicarbonate in a large evaporating dish. After mixing thoroughly, spray with 6M NH_4OH while stirring. Cover with a layer of crushed ice and stir. When the smoke of NH_4Cl has partly subsided, add iced water and stir. Dump this slurry into a large container. Repeat until all has been treated. Neutralize and slowly siphon the suspension into the drain with excess running water. Notify local sewage authority (3).

VIII. REFERENCES

1. Windholz, M., S. Budavari, R.F. Blumetti, and E.S. Otterbein, eds. 1983. The Merck Index, 10th ed., p. 1357. Merck and Co., Inc., Rahway, NJ.
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TITANIUM TETRACHLORIDE (cont.)

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TRIAMINOTRINITROBENZENE

Much of the available data on triaminotrinitrobenzene has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

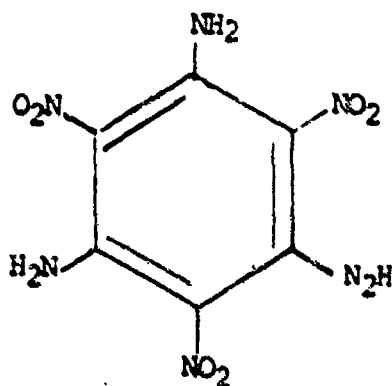
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_3N_6O_6$

Molecular Weight: 258.15 (Estimated)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 3058-38-6

CA Name (9CI): 1,3,5-Benzenetriamine, 2,4,6,-trinitro-

CA Name (8CI): Same

Alternate CAS Registry Number: 67539-61-1

Alternate CA Name (9CI): Benzenetriamine, ar,ar,ar-trinitro-

Other significant synonyms: 1,3,5-Triamino-2,4,6-Trinitrobenzene
s-Triaminotrinitrobenzene, sys-Triaminotrinitrobenzene, 2,4,6-Trinitro-1,3,5-benzenetriamine

TRIAMINOTRINITROBENZENE (cont.)

C. Chemical and Physical Properties

Physical State: Triclinic crystals (1)

Color: Light yellow (1)

Odor: Data not available

Melting Point: Decomposes at 450-451°C (1); 350°C (2)

Solubilities:

Water: Soluble in acids, 20% wt/vol in concentrated sulfuric acid, fluorosulfonic, chlorosulfonic and trifluoromethane sulfonic acids (1).

Nonaqueous Solvents: Soluble in approximately 1% wt/vol in aniline, dimethylformamide, ethylenediamine. Insoluble in benzene, chloroform, ethanol, ether, and glacial acetic acid (1).

Density (Crystal): 1.93 g/cc (1)

Volatility: Not volatile (1)

Vapor Pressure: 10^{-5} torr at 171.3°C 10^{-7} torr at 131.4°C (1)

Heat of Combustion: 735.0 kcal/mol (1)

Stability: Relatively insensitive high explosive (3); excellent thermal stability up to 260-290°C (2).

Flammability: Low; autoignition temperature = 368°C (3)

II. USES

A. Army Unique Use

Currently being processed at Holston AAP for DOE use (4). It is coated with a binder and granulated, then shipped to the Amarillo, Texas DOE facility.

Used in nuclear weapons systems (1).

B. Other Uses

DOE unique (5).

TRIAMINOTRINITROBENZENE (cont.)

III. ANALYTICAL METHODS

A. Best Acceptable Method

An assay method of analysis for TATB using high pressure liquid chromatography was developed by Schaffer. This is primarily designed for production quality control, but could possibly be adapted for trace analysis.

B. Limit of Detection

Data not available

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF TRIAMINOTRINITROBENZENE*

EFFECTS	REFERENCE
Although specific data are not available, the material should be treated as highly toxic by ingestion, inhalation, and skin absorption	(1)

* Information not included in the ARC report.

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of triaminotrinitrobenzene.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Data not available

TRIAMINOTRINITROBENZENE (cont.)

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (6).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (7).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Kaye, Seymour. 1980. Encyclopedia of Explosives and Related Items, Vol. 9, pp. 34-54. PATR2700. US Army Armament Research and Development Command, Dover, NJ.
2. Urbanski, T. 1984. Chemistry and Technology of Explosives, Vol. 4, p. 204. Elmsford, NY.
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TRIETHANOL AMMONIUM NITRATE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_{15}NO_3 \cdot HNO_3$

Molecular Weight: 212.2

Structural Formula: $(HOCH_2CH_2)_3NH^{+1}NO_3^{-1}$

B. Alternate Names and Registry Numbers

CAS Registry Number: 27096-29-3

Deleted CAS Registry Number: 29868-09-5

CA Name (9CI): Ethanol, 2,2',2''-nitrilotris-, nitrate (salt)

CA Name (8CI): Ethanol, 2,2',2''-nitrilotri-, nitrate (salt)

RTECS Number: Data not available

Other Significant Synonyms: Triethanolamine-nitric acid salt;
Triethanolamine nitrate; Triethanolamine mononitrate; TEAN

C. Chemical and Physical Properties

Physical State: Data not available

Color: Data not available

Odor: Data not available

Melting Point: Data not available

Solubilities:

Water: Data not available

Nonaqueous Solvents: Data not available

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

TRIETHANOL AMMONIUM NITRATE (cont.)

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Propellant

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

Kaplan et al. (1) used gas chromatography to monitor soil degradation of TEAN. The free amine was determined with a flame ionization detector (FID) eluted from a Tenax-GC packed column at 260°C. Kaplan et al. also performed GC analysis for the presence of TEAN in the headspace gas in the biodegradation studies. Carbosieve columns with a thermal conductivity detector and temperature programming were used.

B. Limit of Detection

Kaplan et al. reported 175.8 ng as the limit of detection for TEAN as the free amine using the FID.

TRIETHANOL AMMONIUM NITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF TRIETHANOL AMMONIUM NITRATE

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Triethanol ammonium nitrate				No toxicity data located; data on structural analogues and chemical classes follow below	
Nitrates	Human	oral	Large amounts	Dizziness, abdominal cramps, vomiting, bloody diarrhea, weakness, convulsions, and collapse	(2)
			Small repeated doses	May lead to weakness, general depression, headache, and mental impairment	
Triethanol amine	Human	skin	15 mg, 3 days	Mild irritation	(3)
	Rat	oral	8,680 mg/kg	LD ₅₀	(3)
	Rat	oral	9,110 mg/kg	LD ₅₀	(4)
	Rat	oral (feed)	90 days: 0.73 g/kg	Microscopic lesions and deaths	(4)
			0.17 g/kg	Changes in liver and kidney weights	
			0.08 g/kg	No effect	
	Mouse	intra-peritoneal	1,450 mg/kg	LD ₅₀	(3)
	Mouse	oral (feed)	0.03 or 0.3% diet	Significant increases in incidences of females	(4)

TRIETHANOL AMMONIUM NITRATE (cont.)

TABLE IV-1. TOXICITY OF TRIETHANOL AMMONIUM NITRATE (Cont.)

Chemical	Species	Route	Dose/ Duration	Effects	Reference
Triethanol amine cont.)	Guinea pig	oral	8,000 mg/kg	LD ₅₀	(3)
	Rabbit	skin	560 mg, 24 hr	Mild irritation	(3)
	Rabbit	eye	5,620 ug	Severe irritation	(3)
	Rabbit or rat	skin	5 or 10% solution	Not irritating	(4)
N-Nitroso diethanol amine (NDELA)				Triethanolamine may produce, or contain as an impurity, di- ethanolamine, which in the presence of nitrite, nitrate, or nitrogen oxides may lead to the formation of the carcinogen NDELA	(4)
	Rat	drink- ing water	600 - 1,000 mg/kg	Hepatocellular carcinomas	(3)
	Hamster	subcu- taneous	565 mg/kg 2x/wk for over 45 wk; killed at wk 78	Nasal cavity adeno- carcinomas and tracheal tumors	(3)

* Not specified

V. ENVIRONMENTAL EFFECTS

No data available

VI. STANDARDS AND REGULATIONS

No data available

VII. DISPOSAL METHODS

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (5).

B. Alternate Disposal Methods Under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (6).

Disposal practices recommended by the U.S. Navy in their Consolidated hazardous item list for hydroxylamine, the parent compound of hydroxylammonium nitrate, is to return to the supplier (7).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

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5. David Renard, U.S. Army Hazardous and Material Agency, to J. Carl Uhrmacher (personal communication). 1985.

TRIETHANOL AMMONIUM NITRATE (cont.)

6. Forsten, I. 1980. Disposal of Hazardous Toxic Munition Waste. Proceedings of the 1980 National Conference of Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers Division, New York. 440-575.
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TRIETHYLENE GLYCOL DINITRATE

Much of the available data on triethylene glycol dinitrate has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled, A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals. Data reported herein reflects information more recent than that reported by ARC in 1978.

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_6H_{12}N_2O_8$

Molecular Weight: 240.20 (1)

Structural Formula: $O_2NO(CH_2CH_2O)_3ONO_2$

B. Alternate Names and Registry Numbers

CAS Registry Number: 111-22-8

CA Name (9CI): Ethanol, 2,2'-[1,2-ethanediylbis(oxy)]bis-, dinitrate

CA Name (8CI): Triethylene glycol, dinitrate

RTECS Number: YE5500000

Other Significant Synonyms: TEGDN

C. Chemical and Physical Properties

Physical State: Oily liquid (1)

Color: Light yellow (1)

Odor: Data not available

Melting Point: $-19^{\circ}C$ (1)

Solubilities:

Water: Slightly soluble (1).

Nonaqueous Solvents: Very soluble in acetone, ether, and 2:1 ether-ethanol; soluble in carbon disulfide (1).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

TRIETHYLENE GLYCOL DINITRATE (cont.)

Specific Gravity (Liquid): 1.335 (1)

Volatility: 40 mg/cc/hr at 60°C (1)

Vapor Pressure: 0.001 mm at 25°C (1)

Specific Heat: Data not available

Heat of Combustion: 3428 cal/g or 819 kcal/mole (1)

Reactivity: Data not available

Stability: Do not expose to shock, heat, flame or electrostatic discharge (2).

Flammability: Moderate hazard (2); explosive temperature is 223°C.

II. USES

A. Army Unique Use

High explosive (2).

B. Other Uses

Data not available

III. ANALYTICAL METHODS

A. Best Acceptable Method

Malotky and Downes reported a field kit for the analysis of 28 different explosives including TEGDN using thin-layer chromatography.

B. Limit of Detection

Data not available

TRIETHYLENE GLYCOL DINITRATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF TRIETHYLENE GLYCOL DINITRATE*

Species	Route	Dose/Duration	Effects	Reference
Human	NS**	NS	Organic nitrates produce vasodilation, headache, dizziness, weakness, and other signs of cerebral ischemia associated with postural hypotension; may progress to loss of consciousness; drug rash is occasionally produced	(3)
Rat (NMRI:O(SD) Sprague-Daw- ley-derived)	intra- peritoneal	796 mg/kg	Increased plasma activities of alkaline phosphatase, creatine kinase, aspartate aminotransferase, and lactic dehydrogenase	(4)
Rat (NMRI:O(SD) Sprague-Daw- ley-derived)	intra- peritoneal	acute, lethal dose	Convulsions, hyperactivity to auditory and tactile stimuli	(5)
Rat (NMRI:O(SD) Sprague-Daw- ley-derived)	sc	13.0 mmol/kg	Methemoglobin formation, ataxia, lethargy, respiratory depression, violent tremors, hyperactivity to auditory and tactile stimuli	(4)
Guinea pig (FTD:Hartley- derived)	intra- peritoneal	100, 200, and 400 mg/kg daily for 15 d	Decreased food intake and retarded weight gain	(4)
Rabbit (New Zealand)	dermal	21 mmol/kg daily for 3 wk	Death in 2-3 wk, 20% loss in body weight, emaciated appearance	(4)
Rhesus monkey	inhal- ation	2.4 ppm aerosol for 2 or 4 hr	No significant changes in electroencephalograph or visual evoked response; significant increase in Sidman avoidance response rate	(6)

TRIETHYLENE GLYCOL DINITRATE (cont.)

V. ENVIRONMENTAL EFFECTS

No information was found regarding the fate or effects of triethylene glycol dinitrate which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in the EPA TSCA Inventory 1980.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Past Installation Assessment Reports indicate that current methods of disposal of waste explosives and propellants involve open burning, open detonation or hauling by a licensed contractor and landfilling. This has also been confirmed by private communications from the U.S. Army Toxic and Hazardous Materials Agency (USATHAMA), which has the responsibility to review current disposal practices, and to develop plans for future disposal practices (7).

B. Alternate Disposal Practices under Consideration by the Army

Future plans for disposal of waste explosives and propellants are projected to emphasize fluid-bed incineration. This method has been tested successfully by ARRADCOM and is planned for use at installations such as Savanna Army Depot, Tooele Army Depot, and Hawthorne Naval Ammunition Depot (8).

C. Other Disposal Practices Employed

Data not available

VIII. REFERENCES

1. Kaye, Seymour. 1980. Encyclopedia of Explosives and Related Items, Vol. 9, p. T-57. U.S. Army Armament Research and Development Command, Dover, NJ.

TRIETHYLENE GLYCOL DINITRATE (cont.)

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7. David Renard, U.S. Army Toxic and Hazardous Materials Agency, to J. Carl Uhrmacher (personal communication). 1983.
8. Forsten, I. 1980. Disposal of Hazardous Toxic Munition Waste. Proceedings of the 1980 National Conference of Environmental Engineering. New York, July 8-10, 1980. ASCE Environmental Engineers Division, New York. 440-575.

VAT YELLOW 4

Much of the data on Vat Yellow 4 has been reported in a previous study by the Atlantic Research Corporation (ARC) entitled A Preliminary Problem Definition Study of 48 Munitions-Related Chemicals (1). Data reported herein reflects information more recent than that reported by ARC in 1978.

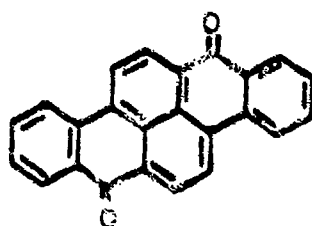
I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $C_{24}H_{12}O_2$

Molecular Weight: 332.25 (1)

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 128-66-5

Deleted CAS Registry Numbers: 39280-74-5, 12772-52-0

CA Name (9CI): Dibenzo[b,def]chrysone-7,14-dione

CA Name (BCI): Same

RTECS Number: H07030000

Other Significant Synonyms: Numerous (1). 3,8:8,9-Dibenzopyrene-5,10-dione

C. Chemical and Physical Properties

Physical State: Solid (1)

Color: Yellow

Odor: Data not available

Melting Point: Data not available

VAT YELLOW 4 (cont.)

Solubilities:

Water: Data not available

Nonaqueous Solvents: Soluble in nitrobenzene, xylene, tetrahydronaphthalene (1); slightly soluble in acetone, alcohol, benzene, chloroform, o-chlorophenol, pyridine, toluene (1).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): Data not available

Volatility: Data not available

Vapor Pressure: Data not available

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Data not available

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Coloring agent to produce yellow smoke (1)

B. Other Uses

Dye

III. ANALYTICAL METHODS

A. Best Acceptable Method

Vat Yellow 4 can be analyzed by column and thin-layer chromatography and ultra violet, visible and fluorescence spectrophotometry. These methods have been used by Pierce and Katz (2) for air pollution analysis.

B. Limit of Detection

Data not available

VAT YELLOW 4 (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF VAT YELLOW 4*

Species	Route	Dose/Duration	Effects	Reference
Rat (Fischer 344)	oral	0, 3,500, or 7,000 ppm in feed for 104 wk	Decreased body weight gain; no significant increases in tumor incidences compared with controls	(3)
Mouse (B6C3F1)	oral	Males: 0, 25,000 or 50,000 ppm; Females: 0, 12,500, or 25,000 ppm in feed for 106 wk	Increased incidence of lymphoma in high-dose males: controls 3/20 (15%), low-dose 7/47 (15%), high-dose 22/50 (44%, P=0.019). Females showed no sig- nificant increases in tumor incidences com- pared with controls	(3)

* Information not included in the ARC report

TABLE IV-2. MUTAGENICITY AND RELATED EFFECTS OF VAT YELLOW 4

Test System	Dose	Effects	Reference
<u>Salmonella</u> <u>typhimurium</u> TA98, TA100, TA1535, TA1537 TA1538	0.1-1,000 ug/plate	Nonmutagenic with or without Aroclor 1254- induced rat liver S9	(4)
<u>Salmonella</u> <u>typhimurium</u>	NS*	Nonmutagenic with or without Aroclor 1254- induced rat or Syrian hamster liver S9	(5)

* Not specified

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of Vat Yellow 4 which would update the Atlantic Research Corporation document.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1980.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for Dye Solution, a related compound used for a related purpose are to dilute with a flammable solvent and to burn in an incinerator equipped with an afterburner (6).

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

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VAT YELLOW 4 (cont.)

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WHITE PHOSPHORUS

I. CHEMICAL AND PHYSICAL DATA

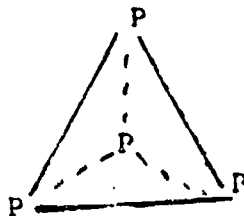
A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: P_4

Atomic Weight: 30.97

Molecular Weight: 123.89

Structural Formula:



B. Alternate Names and Registry Numbers

CAS Registry Number: 7723-14-0*

Deleted CAS Registry Number: 29879-37-6

CA Name (9CI): Phosphorus

CA Name (8CI): Same

RTECS Number: TH3495000, TH3505000, TH3500000

Other Significant Synonyms: Yellow phosphorus

B. Alternate Names and Registry Numbers

CAS Registry Number: 12185-10-3

Deleted CAS Registry Number: 51273-58-6

CA Name (9CI): Phosphorus, mol. (P_4)

CA Name (8CI): Same

RTECS Number: Data not available

WHITE PHOSPHORUS (cont.)

Other significant synonyms: Tetraphosphorus, Phosphorus tetraatomic molecule, Tetrameric phosphorus, molecular phosphorus, Tetraphosphatricyclo-[1.1.0.02,4]butane

*Chemical Abstracts Service assigns the same Registry Number, 7723-14-0 for two forms of elemental phosphorus, white and red.

C. Chemical and Physical Properties

Physical State: Crystalline solid with two allotropic modifications: .alpha. form exists at room temperature as cubic crystals; .beta. form is formed at -79.6°C as hexagonal crystals (1).

Color: Colorless or white, transparent, waxy appearance; darkens on exposure to light (1).

Odor: Data not available

Melting Point: 44.1°C (1)

Boiling Point: 280°C (1)

Solubilities:

Water: One part in 300,000 (1).

Nonaqueous Solvents: 1 g/400 mL absolute alcohol, 1 g/102 mL absolute ether, 1 g/40 mL in chloroform, 1 g/35 mL in benzene, 1 g/80 mL in olive oil, 1 g/60 mL turpentine, 1 g/100 mL almond oil (1); Soluble in anhydrous ammonia and toluene (2).

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density (Crystal): 1.88 g/cc (1); 1.82 g/cc at 20° (2); 1.83 g/cc (3)

Volatility: Very volatile; gives off white fumes and a greenish light when exposed to air in the dark (1)

Vapor Pressure: 0.181 mm Hg (1)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Very reactive, combines directly with halogens and metals, must be kept under water (1).

Stability: Very unstable, will ignite at 30°C in moist air (1).

WHITE PHOSPHORUS (cont.)

Flammability: Very (1), autoignition point: 45°C (3).

II. USES

A. Army Unique Use

Obscurant

B. Other Uses

Rat poison (1)

III. ANALYTICAL METHODS

A. Best Acceptable Method

White phosphorus can be detected by some of the same methods as red phosphorus. For detection of white phosphorus, a photometric detector designed to monitor cold chemiluminescence has been reported by Mielniczuk (4).

B. Limit of Detection

Data not available

WHITE PHOSPHORUS (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF WHITE PHOSPHOROUS

Species	Route	Dose/Duration	Effects	Reference
Human	oral	1,400 ug/kg	LD _{Lo}	(5)
Human	oral	Acute	Gastrointestinal effects including nausea, vomiting, belching may occur within 30 min; death from cardiovascular collapse can occur within 12 hr; a period of apparent recovery lasting about 2 days may occur followed by the return of gastrointestinal distress with hepatic, renal, and cardiovascular effects including jaundice, pitting edema, oliguria, high pulse rate, and low blood pressure; liver and kidney effects observed at death	(6)
Human	inhalation	Chronic	Gastrointestinal distress; phosphorus odor of the breath; slight jaundice; necrosis of bone, particularly the jaw; leukopenia, anemia	(6)
Human	oral	0.2 mg/kg	Minimum toxic dose	(6)
Human	oral	16 mg/kg	Effects on the gastrointestinal tract; coma	(5)
Human	oral	2,600 ug/kg	Effects on the gastrointestinal tract and behavior	(5)
Human	local	NS*	Severe burns of the skin; ocular damage	(6)

* Not specified

WHITE PHOSPHORUS (cont.)

TABLE IV-1. TOXICITY OF WHITE PHOSPHOROUS (Cont.)

Species	Route	Dose/Duration	Effects	Reference
Human	inhalation	100-700 mg/m ³ for less than 15 min	Phosphorus smoke formulations caused reversible pulmonary symptoms and mucous membrane irritation	(7)
Rat	oral	11 ug/kg, days 1-22 of gestation	Effects on fertility	(5)
Rat	oral	3,030 ug/kg	LD ₅₀ ; effects on behavior and the pulmonary system	(5)
Mouse	oral	4,820 ug/kg	LD ₅₀ ; effects on behavior and the pulmonary system	(5)
Rabbit	sub-cutaneous	10 mg/kg	LD _{Lo}	(5)
Dog	oral	50 mg/kg	LD _{Lo}	(5)
Dog	sub-cutaneous	2 mg/kg	LD _{Lo}	(5)
Pig	oral	160 mg/kg	LD _{Lo}	(5)
Duck	oral	3 mg/kg	LD _{Lo} ; convulsions	(5)

* Not specified

WHITE PHOSPHORUS (cont.)

V. ENVIRONMENTAL EFFECTS

Summary of Programmatic Life Cycle Assessment

White phosphorous is reported to be transformed into phosphate salts in the environment by the action of water, air and sunlight. Unburned white phosphorous was observed to burn exposed vegetation in the immediate area of release. White phosphorous transformed into phosphates is rapidly complexed by soil constituents and absorbed by soil particles or biota.

Aquatic toxicity of white phosphorous has been difficult to measure because of its reactivity, rapidly disproportionating to phosphorous and phosphoric acids. White phosphorous dissolved in water is toxic to fresh water aquatic invertebrates and fish. White phosphorous is also toxic to saltwater species, with the Atlantic salmon observed to be the most sensitive. One author cited recommended a water quality criterion of 0.6 ug/L for white phosphorous. Prolonged exposure to elevated phosphorus levels in aquatic system can have adverse affects. Water pH may be lowered in some water systems causing algae blooms and lowering of dissolved oxygen resulting in fish kills.

Toxicity was also reported in black ducks and mallards. Sublethal effects of white phosphorous were reported for white phosphorous levels in smokes above 1000 milligrams per cubic meter and animals could receive lethal doses of elemental phosphorus if they ingested unreacted materials containing white phosphorous (8).

A. Environmental Fate

A1. Transport

A1a. Adsorption -- Data not available

A1b. Volatilization -- Data not available

A1c. Leachability -- Data not available

A1d. Bioaccumulation -- Radioactive phosphorus has been concentrated by waterfowl up to 75,000 times and by aquatic life by factors up to 850,000. Cod and other marine fish concentrate up to 1,000 times (3).

A2. Transformation -- Data not available

A2a. Biodegradation -- Data not available

A2b. Hydrolysis -- See A2c.

A2c. Photolysis -- Data not available

A2d. Other chemical reaction -- Burns spontaneously in air (see Stability).

WHITE PHOSPHORUS (cont.)

A2e. Half-life -- Although there are no definitive published reports on the kinetics of oxidation of elemental phosphorus in water, it appears that the rate is highly dependent on the degree of dispersion. At concentration (about 10 ug/L) well below the accepted solubility limit of 3 mg/L (dissolved oxygen concentration unspecified), elemental phosphorus disappears by a first order process, with a half-life of 2 hours at about 10°C, 0.85 hour at 30°C. At concentrations (50 to 100 mg/L) well above the solubility limit, with a dissolved oxygen concentration of 6 to 7 mg/L, the same reaction has a half-life of 80 hours at 30°C and 240 hours at 0°C. The relatively small temperature effect combined with the large inverse concentration effect is consistent with a diffusion-controlled process. The oxidation of colloidal phosphorus in sea water is reported to be measurably slower than in fresh water, suggesting that the high salt content brings about agglomeration of the phosphorus particles (3).

B. Effects on animals

- B1. Avian species -- Data not available
- B2. Mammalian wildlife species -- Data not available
- B3. Terrestrial invertebrates -- Data not available
- B4. Reptiles -- Data not available
- B5. Amphibians -- Data not available
- B6. Microorganisms, aquatic and soil -- Data not available
- B7. Aquatic species, fish and invertebrates -- Data not available

C. Effects on plants

- C1. Phytotoxicity -- Data not available
- C2. Uptake -- Data not available
- C3. Metabolism -- Data not available

VI. STANDARDS AND REGULATIONS

A. Health

TLV: TWA 0.1 mg/m³; STEL 0.3 mg/m³ for 15 minute exposure (3).

WHITE PHOSPHORUS (cont.)

B. Environmental

Reported in EPA TSCA Inventory 1980.

Phosphorus has a statutory reportable quantity (RQ) of 1 lb. under the Comprehensive Environmental Response, Compensation and Liability Act. The National Response Center must be notified immediately when there is a release of this compound in an amount equal to or greater than the reportable quantity (9).

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

A recent programmatic life cycle environmental assessment indicates that incineration is the preferred method for disposal of smoke/obscurant munitions. Munitions containing phosphorous would be incinerated in a unit equipped with afterburner and a scrubber (8).

B. Alternate Disposal Practices Under Consideration by the Army

AMCCOM anticipates future waste smoke munitions will be demilitarized and white phosphorous recovered as phosphoric acid (8).

C. Other Disposal Practices Employed

Data not available

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ZINC NAPHTHENATE

I. CHEMICAL AND PHYSICAL DATA

A. Structural and Chemical Formulas and Molecular Weight

Chemical Formula: $\text{Zn}(\text{C}_6\text{H}_5\text{COOH})_2$

Molecular Weight: 319.7

Structural Formula: Naphthene is a term used in the petroleum industry to denote five- and six-carbon cycloparaffins and their alkyl derivatives, found in crude petroleum. Sometimes used to include polycyclic members found in higher boiling fractions (1). This is not a unique chemical substance (CAS), but represents the Zinc (+2) salts of mixed naphthene carboxylic acids.

B. Alternate Names and Registry Numbers

CAS Registry Number: 12001-85-3

CA Name (9CI): Napthenic acids, zinc salts

RTECS Number: QK9275000

Other Significant Synonyms: Zinc oversol

C. Chemical and Physical Properties

Physical State: Mixture, Viscous, basic liquid (with 8-10% Zn) or basic solid (with 16% Zn) (1)

Color: Amber (1)

Odor: Data not available

Melting Point: Not defined for a mixture

Solubilities:

Water: Data not available

Nonaqueous Solvents: Very soluble in acetone. (1)

Octanol Water Partition Coefficient: Data not available

Hygroscopicity: Data not available

Density: Data not available

Volatility: Data not available

Vapor Pressure: Data not available

ZINC NAPHTHENATE (cont.)

Specific Heat: Data not available

Heat of Combustion: Data not available

Reactivity: Combustible (1)

Stability: Data not available

Flammability: Data not available

II. USES

A. Army Unique Use

Military anti-mildew agent

B. Other Uses

Drier and wetting agent in paints, varnishes and resins; insecticide, fungicide, and mildew preventive; wood preservative; waterproofing textiles; insulating materials (1).

III. ANALYTICAL METHODS

A. Best Acceptable Method

No methods were found for either zinc naphthenate or naphthenic acid in searching the Chemical Abstracts System back to 1967. Zinc can be analyzed by either atomic absorption spectroscopy or atomic emission spectrometry. Recently, a method was reported to enhance the detection of zinc by simultaneous inductively coupled plasma atomic emission spectrometry by Hee et al. (2).

B. Limit of Detection

The lower determination range for zinc reported by Hee et al. is 0.01-1.0 microgram/milliliter. The apparent linear range is 2.0 to 250 microgram/milliliter (2).

C. High Performance Liquid Chromatography

Data not available

ZINC NAPHTHENATE (cont.)

IV. HEALTH EFFECTS

TABLE IV-1. TOXICITY OF ZINC NAPHTHENATE

Species	Route	Dose/Duration	Effects	Reference
Human	oral	NS*	Some soluble zinc salts cause nausea and vomiting	(3)
Human	eyes, skin	NS	Naphthenic acids are irritants	(4)
Rat	oral	4,920 mg/kg (in lard)	LD ₅₀	(5)
Rat	oral	6,000 mg/kg once	Practically nontoxic	(6)
NS	NS	NS	Low toxicity	(1)

* Not specified

V. ENVIRONMENTAL EFFECTS

No information was found regarding the environmental fate or effects of zinc naphthenate.

VI. STANDARDS AND REGULATIONS

A. Health

Data not available

B. Environmental

Reported in EPA TSCA Inventory 1980.

VII. DISPOSAL

A. Current Recommended Army Disposal Practices

Disposal practices recommended by the U.S. Navy in their Consolidated Hazardous Item List for Copper Naphthenate, a related compound used for a related purpose, are to turn in to a pesticide collection center, to the original supplier or to a commercial waste disposal service (7).

ZINC NAPHTHENATE (cont.)

B. Alternate Disposal Practices Under Consideration by the Army

Data not available

C. Other Disposal Practices Employed

Data not available

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